Electronic Supplementary Information

DFT and Machine Learning Insights into Ru(II) Complex-Catalyzed Transfer Hydrogenation

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1. The Comparison of Free Energy Barriers Using Different Functionals

Table S1. The comparison of free energy barrier using different functionals (kcal/mol).

Structural	M06-L	B3LYP-D3(BJ)	WB97XD	M06	TPSSH
Int0	0.0	0.0	0.0	0.0	0.0
Int1	2.6	3.8	3.5	3.5	2.8
D-TS3	28.5	32.7	32.6	30.6	31.7
D-Int2	7.4	10.5	9.6	8.7	9.5

In order to select appropriate functional for our calculation, we compare a series of functionals which are widely used in the computational studies relevant to the dehydrogenation step in transfer hydrogenation. The rate-determining transition states and intermediates were calculated using different functionals. The results are shown in Table S1. The relative reaction activation energy and mechanism selectivity calculated by different functionals is basically the same trend. Based on these results, we chose M06-L as the functional considering the computational expense and accuracy.

2. The Calculation Details of Standard State Correction

As for the room temperature (298.15 K), the molar volume of an ideal gas in the gas phase standard state (298.15 K, 1 atm):

$$V_m = \frac{RT}{P} = \frac{8.314 \times 298.15}{101325} = 0.02246\ \mathrm{m^3/mol} = 24.46\ \mathrm{L/mol}$$

The free energy change of the process of compressing 1M ideal gas into 1M solution concentration in the standard state:

$$\Delta G_{1\mathrm{atm}\rightarrow 1\mathrm{M}}^{298.15\mathrm{K}} = RTln(\frac{V_a}{V_b}) = \frac{8.314 \times 298.15 \times \ln(24.46)}{1000} = 7.92\ \mathrm{KJ/mol} = 1.89\ \mathrm{kcal/mol}$$

As for the experimental condition (358.15 K), the molar volume of an ideal gas in the gas phase state (358.15 K, 1 atm):

$$V_m = \frac{RT}{P} = \frac{8.314 \times 358.15}{101325} = 0.02939\ \mathrm{m^3/mol} = 29.39\ \mathrm{L/mol}$$

The free energy change of the process of compressing 1M ideal gas into 1M solution concentration in the standard state:

$$\Delta G_{1\mathrm{atm}\rightarrow 1\mathrm{M}}^{358.15\mathrm{K}} = RTln(\frac{V_a}{V_b}) = \frac{8.314 \times 358.15 \times \ln(29.39)}{1000} = 10.07\ \mathrm{KJ/mol} = 2.41\ \mathrm{kcal/mol}$$

Therefore, a correction factor of 2.41 kcal/mol was applied for the standard state change from 1 atm to 1 M.

3. CREST Conformational Analysis of Representative Catalyst Intermediates

Table S2. CREST conformational analysis of representative catalyst intermediates

Conformer	Δ*E*(kcal/mol)	HOMO	HOMO–LUMO gap	Dipole
150-Int0-1	0.00	-9.1558	2.1777	3.2277
150-Int0-2	0.11	-9.1555	2.1791	3.2505
150-Int0-3	0.11	-9.1555	2.1791	3.2508
150-Int0-4	0.16	-9.1926	2.2101	3.8832
150-Int0-5	0.00	-9.1558	2.1777	3.2261
207-Int0-1	0.00	-8.9768	2.0466	3.8019
207-Int0-2	0.00	-8.9768	2.0466	3.8019
207-Int0-3	0.00	-8.9768	2.0466	3.802
207-Int0-4	0.00	-8.977	2.0468	3.802
207-Int0-5	0.01	-8.9697	2.0351	3.8291
93-Int0-1	0.25	-8.9188	2.018	4.1862
93-Int0-2	0.25	-8.9188	2.018	4.1863
93-Int0-3	0.25	-8.9188	2.018	4.1863
93-Int0-4	0.25	-8.9188	2.018	4.1861
93-Int0-5	0.00	-8.8913	2.024	3.9428
51-Int0-1	0.41	-8.8758	2.0300	4.2896
51-Int0-2	0.41	-8.8761	2.0302	4.2898
51-Int0-3	0.41	-8.8758	2.0300	4.2897
51-Int0-4	0.17	-8.8723	2.0313	4.3636
51-Int0-5	0.00	-8.8723	2.0411	4.2830
134-Int0-1	1.57	-9.0625	2.2019	4.1733
134-Int0-2	1.57	-9.0625	2.2019	4.1719
134-Int0-3	0.64	-8.9585	2.1388	4.0036
134-Int0-4	0.00	-9.0361	2.1853	4.2262
134-Int0-5	0.00	-9.0364	2.1856	4.2258
191-Int0-1	1.48	-8.8652	2.0615	4.0239
191-Int0-2	0.76	-8.7664	2.0098	3.7922
191-Int0-3	0.02	-8.8611	2.0588	4.0492
191-Int0-4	0.00	-8.8562	2.0594	4.018
191-Int0-5	0.59	-8.7778	2.0123	3.7325
77-Int0-1	1.64	-8.8162	2.0302	3.9236
77-Int0-2	0.20	-8.7618	2.0221	3.8773
77-Int0-3	0.00	-8.7964	2.0308	3.9578
77-Int0-4	0.00	-8.7961	2.0308	3.9569
77-Int0-5	0.00	-8.7961	2.0305	3.9573
3-Int0-1	1.44	-8.8505	2.0583	4.7656
3-Int0-2	1.23	-8.8298	2.0534	4.6271

3-Int0-3	1.64	-8.8154	2.0498	4.4016
3-Int0-4	1.78	-8.8124	2.0498	4.3087
3-Int0-5	0.00	-8.7879	2.0455	4.4867

As shown in Table S2, the relative energies of the optimized conformers are generally within ~2 kcal mol^{-1}, and the variations in the electronic descriptors (HOMO energy, HOMO-LUMO gap, and dipole moment) are very small among the conformers of the same catalyst. Representative ball-and-stick structures of the conformers are shown in Figures S1 and S2.

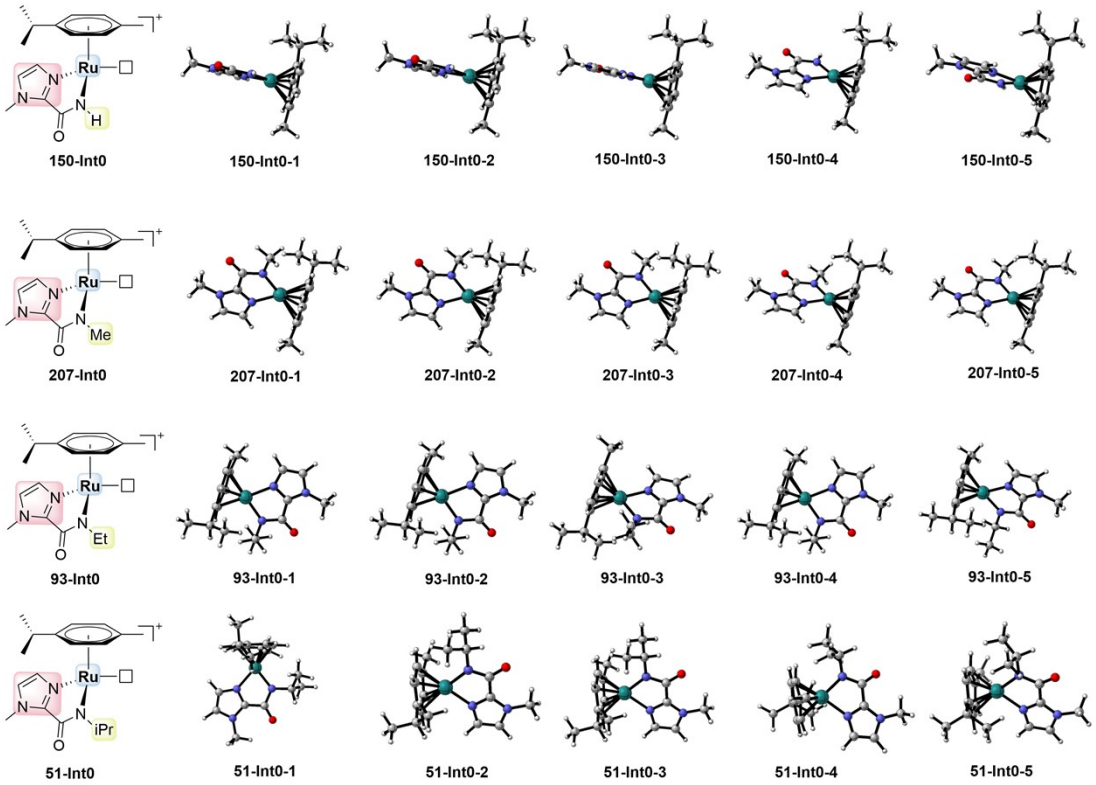


Figure S1. Representative ball-and-stick structures of the conformers

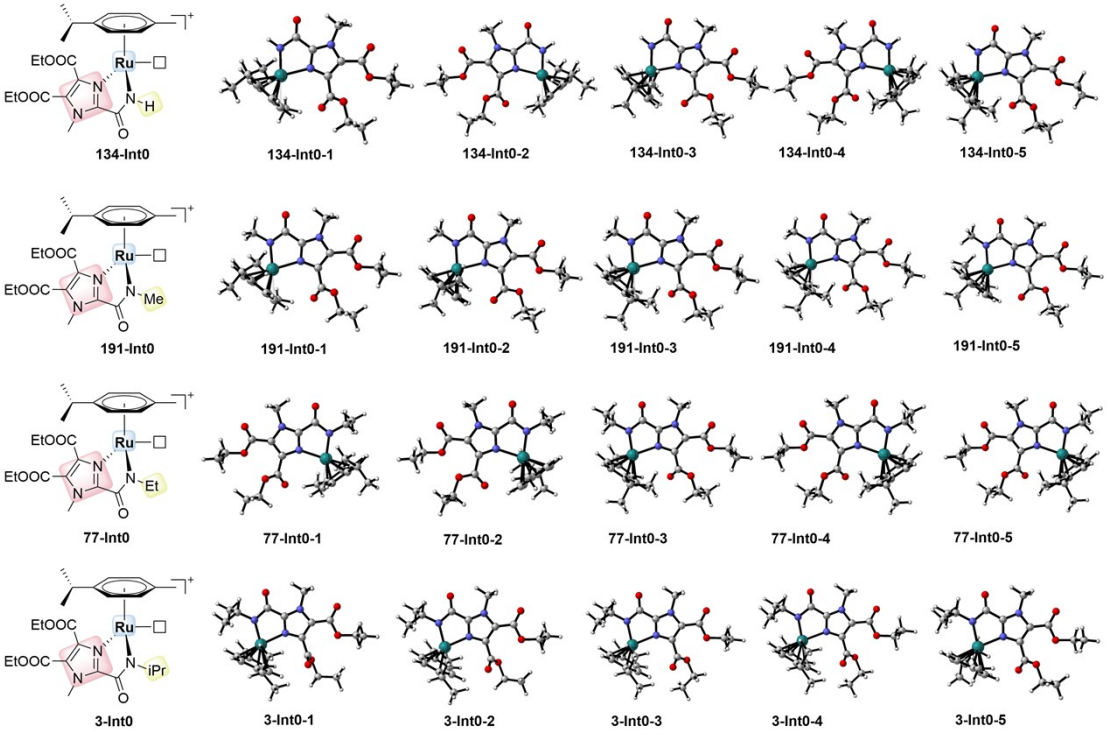


Figure S2. Representative ball-and-stick structures of the conformers

4. Hyperparameter Optimization Grid and Optimal Values for the RF Model

Table S3. Hyperparameter optimization grid and optimal values for the random forest model

Hyperparameter	Optimization grid	Optimal value
Bootstrap	True, False	True
Max Depth	5, 10, None	5
Min Samples Leaf	1, 2, 4	2
Min Samples Split	2, 5, 10	2
N Estimators	100, 300, 500	100

5. Performance Metrics of the RF Model on the Training Set, Independent Test Set, and 5-Fold Cross-Validation

Table S4. Performance metrics of the RF model on the training set, independent test set, and 5-fold cross-validation

Metric	Training set	Test set	5-Fold CV (mean ± std)
R^2	0.8917	0.6368	0.6614 ± 0.0529
RMSE / (kcal·mol^{-1})	0.9515	1.7289	1.6616 ± 0.0918
MAE / (kcal·mol^{-1})	0.7703	1.4220	1.3314 ± 0.0742

6. Relative Energies and Catalytic Cycle of Ru-iPr Enantiomers

Figure S3. The free energy diagram of key intermediates for the Ru-iPr enantiomers

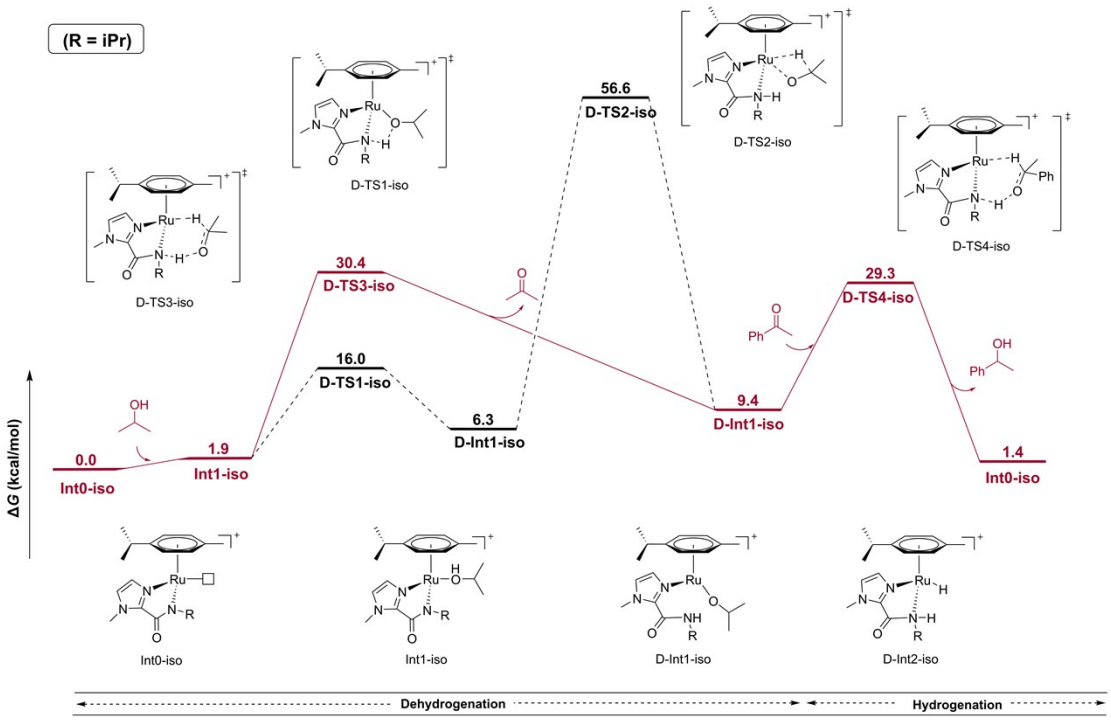
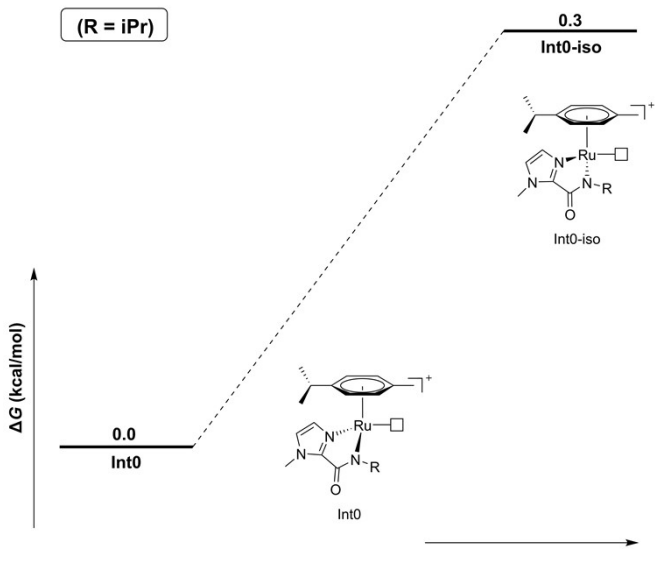


Figure S4. The free energy diagram of the catalytic cycle starting from Int0-iso



The experimental crystal structure of Ru-iPr (CCDC 2480402) is racemic, with both enantiomers present in the system. In the calculations, both configurations were considered. As shown in Figure S2, the key intermediates corresponding to the two enantiomers (Int0 and Int0-iso) have very similar Gibbs free energies (ΔG = 0.3 kcal/mol). The full reaction pathway was also computed for the slightly higher-energy Int0-iso configuration (Figure S3), which shows a rate-determining step barrier of 30.4 kcal/mol, slightly higher than that of the lower-energy Int0 configuration. Since the difference in reaction barriers between the two enantiomers is very small (< 1 kcal/mol), the lower-energy Int0 configuration was selected for detailed mechanistic analysis.

7. The Free Energy Diagram of the tBu-Substituted Ru Catalytic Cycle

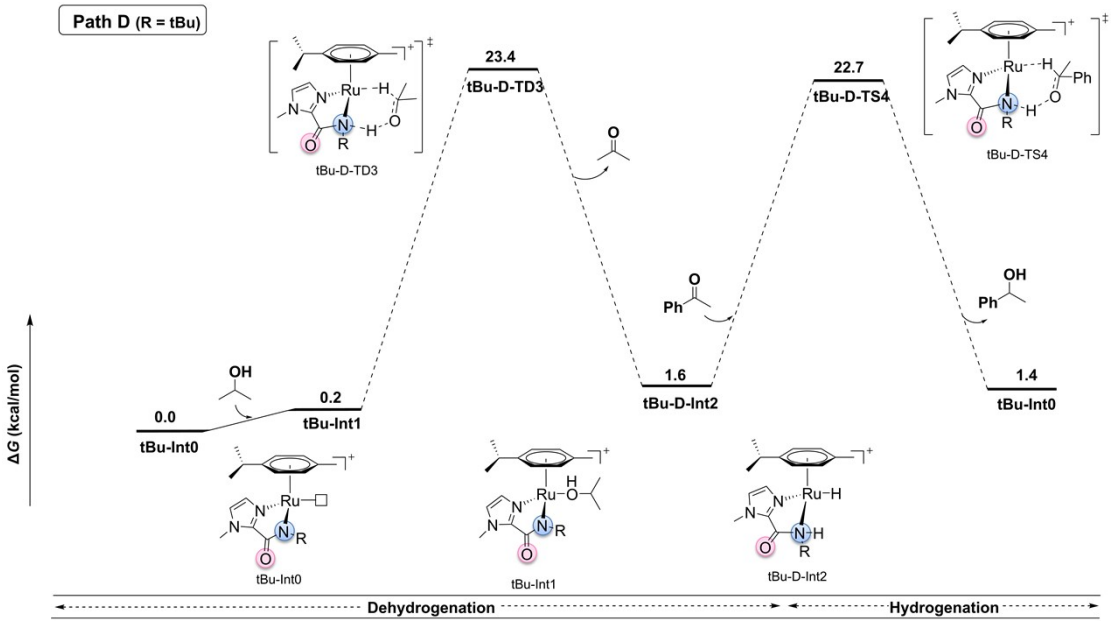


Figure S5. The free energy diagram of the catalytic cycle for the tBu-substituted Ru catalyst

The calculations were primarily performed using the iPr-substituted model because Ru-iPr has a high-quality experimental crystal structure (CCDC 2480402), ensuring the reliability of the initial conformations. To verify the generality of the mechanism, calculations were also performed with the tBu-substituted catalyst. The results show that the reaction barrier for the tBu model is 23.4 kcal·mol^{-1}, which is reasonably close to that of the iPr model (28.5 kcal·mol^{-1}). The corresponding free energy diagram is shown in Figure S4.

8. The DFT Calculated Energies of all Optimized Structures

Table S5. The DFT calculated energies of all optimized structures

Species	**Gc**	**G(gas)**	**Esp + Sol**	**Final G**
	hatree	**hatree**	**hatree**	**hatree**
acetone	0.049178	-192.937059	-193.212225	-193.159206
isopropanol	0.073819	-194.109504	-194.410240	-194.332580
acetophenone	0.096525	-384.472408	-384.993323	-384.892958
phenylethanol	0.119093	-385.640915	-386.186991	-386.064057
Int0	0.346092	-1034.766695	-1036.232643	-1035.882711
Int1	0.447291	-1228.883245	-1230.662289	-1230.211157
D-TS3	0.439362	-1228.841170	-1230.613085	-1230.169883
D-TS1	0.445095	-1228.864301	-1230.637372	-1230.188436
D-Int1	0.447809	-1228.870211	-1230.647036	-1230.195386
D-TS2	0.442680	-1228.773545	-1230.566718	-1230.120198
D-Int2	0.364440	-1035.931941	-1037.412514	-1037.044233
D-TS4	0.485407	-1420.381187	-1422.395751	-1421.906503
B-TS1	0.446579	-1228.838245	-1230.624961	-1230.174541
B-Int1	0.446186	-1228.848803	-1230.636677	-1230.186651
B-TS2	0.443908	-1228.810434	-1230.591248	-1230.143500
B-TS3	0.439289	-1228.807574	-1230.579442	-1230.136312
B-Int2	0.364427	-1035.892862	-1037.383917	-1037.015650
B-TS4	0.486061	-1420.346404	-1422.361058	-1421.871156
C-TS4	0.439262	-1228.837556	-1230.602562	-1230.159460
C-TS1	0.443344	-1228.833470	-1230.600828	-1230.153643
C-Int1	0.447326	-1228.860947	-1230.636878	-1230.185712
C-TS2	0.442309	-1228.801004	-1230.570306	-1230.124156
C-TS3	0.440746	-1228.827843	-1230.595921	-1230.151334
C-Int2	0.365674	-1035.932192	-1037.412377	-1037.042863
C-TS5	0.485401	-1420.381192	-1422.395748	-1421.906507

A-Int1	0.445279	-1228.875272	-1230.649831	-1230.200712
A-TS3	0.439460	-1228.830356	-1230.595703	-1230.152402
A-TS1	0.442983	-1228.845962	-1230.618126	-1230.171303
A-Int2	0.444428	-1228.846044	-1230.623322	-1230.175054
A-TS2	0.438467	-1228.777164	-1230.543651	-1230.101344
A-Int3	0.360908	-1035.907436	-1037.385549	-1037.020800
A-TS4	0.490757	-1420.366691	-1422.379382	-1421.884784
Int0-wb97xd	0.351829	-1034.555437	-1036.230789	-1035.875120
Int1-wb97xd	0.452266	-1228.656230	-1230.658266	-1230.202160
D-TS3-wb97xd	0.447660	-1228.608741	-1230.607184	-1230.155684
D-Int2-wb97xd	0.372327	-1035.730318	-1037.409293	-1037.033126
Int0-TPSSH	0.344006	-1034.892107	-1036.227690	-1035.879843
Int1-TPSSH	0.443236	-1229.042734	-1230.655114	-1230.208037
D-TS3-TPSSH	0.438151	-1229.000167	-1230.603866	-1230.161874
D-Int2-TPSSH	0.364829	-1036.058006	-1037.406769	-1037.038099
Int0-m06	0.344093	-1034.107096	-1036.230515	-1035.882582
Int1-m06	0.444868	-1228.118282	-1230.658236	-1230.209528
D-TS3-m06	0.436331	-1228.076484	-1230.606645	-1230.166473
D-Int2-m06	0.363823	-1035.270640	-1037.409800	-1037.042137
Int0-b3lyp	0.342723	-1034.947736	-1036.227857	-1035.881293
Int1-b3lyp	0.444484	-1229.115556	-1230.656125	-1230.207800
D-TS3-b3lyp	0.439042	-1229.075672	-1230.604595	-1230.161713
D-Int2-b3lyp	0.365457	-1036.119618	-1037.407267	-1037.037969

- The and $\mathbf{G_C}$ designate the Gibbs Free Energy at the M06-L/def2-SVP level.
- The and **G(gas)** designate Gibbs Free Energy in the gas phase at the M06-L/def2-SVP level.
- The $\mathbf{E_{SP} + G_{SOL}}$ designates the sum of single point energy at the M06-L/def2-TZVP level and the solvation free energy calculated by SMD continuum solvent mode.
- The **Final G** designates the sum of $\mathbf{E_{SP} + G_{SOL}}$ and $\mathbf{G_C}$.

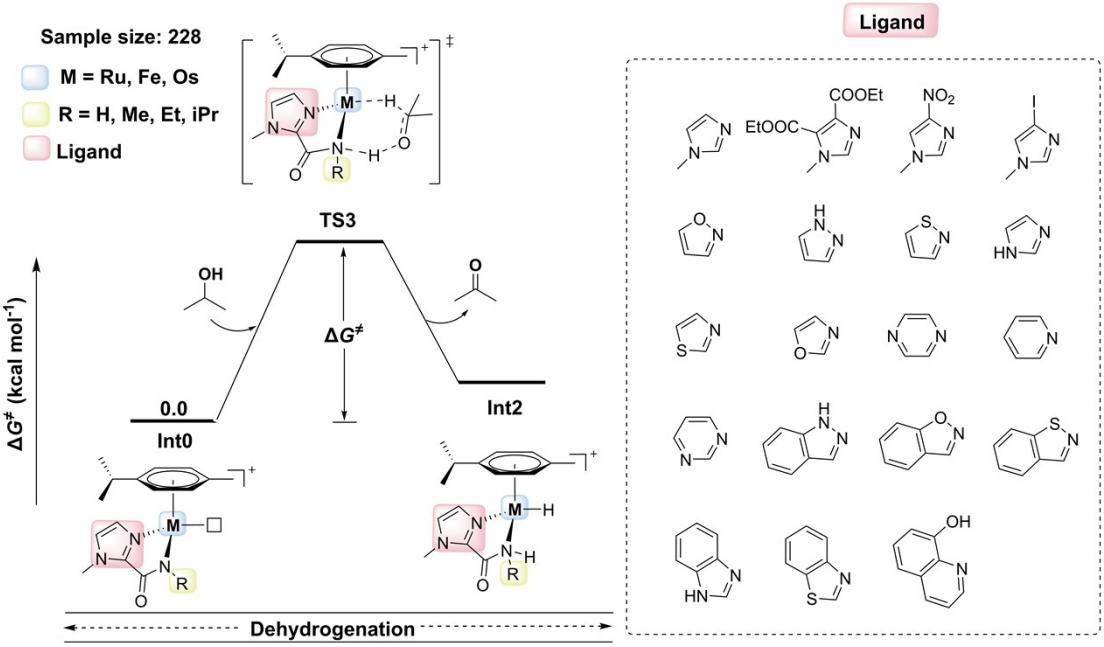


Figure S6. Machine learning sample dataset

9. Machine Learning Sample Dataset

As shown in the figure S6, the machine learning dataset contains 228 samples. To distinguish between different samples, they are named sequentially in the format of **1-Int0**, **1-TS3**, **1-Int2**, **2-Int0**, **2-TS3**, **2-Int2**, ..., **228-Int0**, **228-TS3**, **228-Int2**.

Table S6. Machine learning sample dataset

Species	HOMO	gap	qN2	qM	Dipole	polarizability	$\Delta G^{\neq}$	$\Delta G^{\neq}$(Int2)
1-Int0	-8.6685	1.4158	-0.5516	0.2246	4.4666	321.43	27.4	6.9
2-Int0	-8.7985	2.3772	-0.625	0.3495	3.8571	290.959	35.9	9.7
3-Int0	-8.8081	2.0485	-0.5918	0.1897	4.4695	329.72	28.2	8.3
4-Int0	-8.9749	1.3921	-0.5524	0.213	1.8574	252.6017	26.5	3.1
5-Int0	-9.1063	2.212	-0.6267	0.3452	1.7882	328.4727	30.3	8.6
6-Int0	-9.1226	2.0049	-0.5932	0.174	1.363	261.2037	28.5	7.7
7-Int0	-8.7115	1.4044	-0.5532	0.2267	0.8205	267.0453	25.2	4.4
8-Int0	-8.8355	2.3347	-0.6274	0.3599	0.5534	260.4373	32.9	9.3
9-Int0	-8.8282	1.9856	-0.5942	0.2028	0.9441	274.0273	29	7.9
10-Int0	-9.0614	1.4106	-0.5693	0.2087	4.1652	223.1697	26.1	5.2
11-Int0	-8.881	1.4449	-0.5674	0.2332	6.1795	225.807	26	4.2
12-Int0	-8.9964	1.4449	-0.5598	0.2403	4.1372	233.8973	26.8	5.4
13-Int0	-8.8538	1.4395	-0.558	0.2154	4.3164	223.8827	27	6.6
14-Int0	-9.1164	1.4566	-0.5639	0.2183	5.3537	219.5243	26.9	6.4
15-Int0	-9.029	1.4642	-0.5616	0.2269	5.0993	233.2433	26	5.8
16-Int0	-8.9321	1.5108	-0.5545	0.2408	4.793	242.129	26.7	5.7
17-Int0	-8.5117	1.2738	-0.5221	0.2119	5.836	293.341	28.8	4.3
18-Int0	-8.8636	1.3445	-0.5686	0.2098	3.7452	278.315	25.3	4.3
19-Int0	-8.6968	1.3464	-0.5672	0.2354	5.6456	281.2093	25.7	3.8
20-Int0	-8.7966	1.3728	-0.5584	0.2426	3.6372	289.1997	26.5	5.1
21-Int0	-9.0687	1.5179	-0.5507	0.2426	6.299	238.358	26.9	6.1
22-Int0	-8.7411	1.4349	-0.5573	0.2189	4.0554	236.7013	27.1	6.3
23-Int0	-9.2111	1.517	-0.556	0.2393	5.2579	238.567	26.7	5.9
24-Int0	-8.7057	1.3372	-0.5518	0.2216	3.0347	274.74	27.2	6.6
25-Int0	-8.8753	1.3796	-0.5566	0.2308	5.0001	281.9187	24.6	3.2
26-Int0	-9.1789	2.1375	-0.6342	0.3655	4.1233	278.9637	31.9	9

27-Int0	-9.1792	1.9301	-0.6039	0.1924	4.3887	231.573	28.9	7.8
28-Int0	-8.989	2.3146	-0.6342	0.3533	6.2966	231.2777	31.3	8.2
29-Int0	-8.9822	2.0049	-0.6022	0.2056	6.5217	201.8107	26.9	6.6
30-Int0	-9.133	2.1742	-0.6272	0.3945	4.3353	233.99	34.3	10.3
31-Int0	-9.1365	1.9943	-0.5986	0.232	4.5027	234.779	30.2	8.9
32-Int0	-8.9928	2.3875	-0.6328	0.3632	4.4611	242.021	32.6	9.8
33-Int0	-8.9841	2.0417	-0.599	0.1963	4.4858	242.1477	28.9	8.3
34-Int0	-9.2483	2.3233	-0.6364	0.3646	5.2618	231.1753	32.2	8.7
35-Int0	-9.2404	2.0341	-0.6033	0.196	5.6924	232.466	28.6	8.7
36-Int0	-9.1705	2.2517	-0.631	0.3505	5.0143	226.677	31.1	8.3
37-Int0	-9.1727	2.0278	-0.5998	0.198	5.4253	227.9083	28.1	7.4
38-Int0	-9.1036	2.316	-0.6234	0.3338	4.915	240.9477	32.2	10.1
39-Int0	-9.1082	2.1032	-0.5947	0.199	5.0681	241.9303	28	7.1
40-Int0	-8.6715	2.1192	-0.5985	0.3589	6.0427	249.7037	33.6	7.7
41-Int0	-8.6429	1.861	-0.5664	0.1658	6.0958	250.2087	32	6.7
42-Int0	-8.9697	2.024	-0.6343	0.3643	3.6662	267.9553	31.6	8
43-Int0	-8.9743	1.8379	-0.6046	0.1919	4.0038	268.7963	28.5	6.5
44-Int0	-8.8834	2.3875	-0.632	0.3584	4.2729	245.649	30.2	7.3
45-Int0	-8.7855	2.1315	-0.6355	0.3523	5.5908	254.376	30.4	6.9
46-Int0	-8.7629	1.8411	-0.6038	0.207	5.9768	254.8787	26.8	5.4
47-Int0	-8.9242	2.0866	-0.6274	0.3948	3.6399	290.7267	33.1	9.8
48-Int0	-8.9172	1.892	-0.5989	0.2352	3.9552	289.624	29.4	7.6
49-Int0	-9.2285	2.2441	-0.6238	0.3296	6.2889	298.5137	33.1	9.7
50-Int0	-9.229	2.073	-0.5953	0.1976	6.6064	209.8383	28.9	8
51-Int0	-8.875	2.0387	-0.5993	0.1973	4.2222	246.0637	28.1	7.2
52-Int0	-9.3702	2.1603	-0.6239	0.3271	5.0199	245.7423	32.2	8.9
53-Int0	-9.3705	2.0373	-0.5948	0.1923	5.5833	297.9843	28.5	7
54-Int0	-8.8279	2.2588	-0.6261	0.366	3.4839	244.2573	33.5	11.6
55-Int0	-8.8208	1.9238	-0.592	0.2053	3.4641	245.877	29.9	9.8
56-Int0	-8.9958	2.1619	-0.6254	0.3647	4.9464	281.3513	31.1	8.3
57-Int0	-9.0002	1.935	-0.5933	0.2113	5.3304	245.5497	28.1	6.8
58-Int0	-8.7297	1.4229	-0.5591	0.2169	4.6514	309.8133	31.71	10.24
59-Int0	-8.9841	1.3695	-0.5529	0.2109	2.1308	242.4387	29.34	8.38
60-Int0	-8.7302	1.3842	-0.5551	0.2244	1.1142	256.3337	30.43	8.91

61-Int0	-9.0867	1.3755	-0.5765	0.2008	3.4683	211.454	29.8	8.26
62-Int0	-8.9106	1.4234	-0.5729	0.2194	5.504	214.207	29.58	8.83
63-Int0	-9.0358	1.4332	-0.5658	0.2276	3.6388	222.5973	32.08	10.01
64-Int0	-8.9093	1.4441	-0.5639	0.2048	3.6172	212.6123	30.15	9.99
65-Int0	-9.1705	1.4504	-0.5697	0.2073	4.9027	208.1683	29.91	9.37
66-Int0	-9.0622	1.4398	-0.5666	0.2163	4.6426	221.6143	30.38	9.65
67-Int0	-8.9517	1.47	-0.5594	0.2315	4.1563	230.6073	30.57	11.02
68-Int0	-8.5651	1.3021	-0.5379	0.2081	5.2351	281.5067	28.6	7.38
69-Int0	-8.8845	1.3075	-0.5753	0.2009	3.337	266.2493	29.81	7.95
70-Int0	-8.7139	1.3355	-0.5691	0.2293	5.5905	270.5613	28.4	6.56
71-Int0	-8.8426	1.3736	-0.5644	0.227	3.3773	277.3213	31.39	9.11
72-Int0	-9.0902	1.4713	-0.5566	0.2339	5.8554	226.887	30.75	10.57
73-Int0	-9.2214	1.4632	-0.5617	0.2303	5.0879	227.0573	30.46	9.27
74-Int0	-8.7972	1.4395	-0.563	0.2068	3.3581	225.3767	30.63	10.48
75-Int0	-8.7275	1.3241	-0.554	0.2192	2.8752	264.0357	30.28	10.93
76-Int0	-8.8916	1.3614	-0.5561	0.2299	4.8843	271.3703	28.27	8.2
77-Int0	-8.8712	2.0762	-0.5984	0.2057	4.3773	318.2667	33.42	12.94
78-Int0	-9.1477	1.9921	-0.5914	0.1874	1.6486	250.395	31.28	11.86
79-Int0	-8.8508	1.9769	-0.5929	0.2149	1.125	263.1287	32.08	10.94
80-Int0	-9.2513	1.9467	-0.6086	0.2136	3.749	220.0007	32.38	11.61
81-Int0	-9.053	2.0264	-0.607	0.2226	5.8889	223.1883	30.54	8.98
82-Int0	-9.1879	1.9927	-0.6023	0.2503	3.9475	231.034	32.78	10.36
83-Int0	-9.0587	2.0662	-0.6043	0.2176	3.7418	220.9967	31.64	10.93
84-Int0	-9.3147	2.0512	-0.6087	0.2176	5.1936	216.423	32.03	10.93
85-Int0	-9.2418	2.0436	-0.6047	0.2176	4.9575	230.2173	31.64	10.96
86-Int0	-9.1667	2.1029	-0.6008	0.2179	4.4315	238.69	31.98	11.7
87-Int0	-8.5651	1.3021	-0.5379	0.2081	5.2351	281.5067	28.6	7.38
88-Int0	-9.05	1.8683	-0.6084	0.2143	3.609	275.3257	32.22	10.78
89-Int0	-8.8089	1.8392	-0.6091	0.2271	5.5476	278.9267	30.62	8.41
90-Int0	-8.9689	1.901	-0.6018	0.2503	3.629	286.4097	33.03	11.55
91-Int0	-9.293	2.0741	-0.602	0.2163	6.1406	234.4537	31.28	10.26
92-Int0	-9.4266	2.0305	-0.6016	0.2122	5.3241	234.268	31.76	10.66
93-Int0	-8.9476	2.0632	-0.6045	0.2196	3.4983	234.095	31.79	11.7
94-Int0	-8.8766	1.9244	-0.5973	0.2307	2.8978	271.052	32.31	12.51

95-Int0	-9.0274	1.9238	-0.5906	0.224	5.2703	279.94	31.64	10.45
96-Int0	-8.8837	2.4297	-0.6287	0.3713	3.6618	272.534	36.29	14.16
97-Int0	-9.127	2.1864	-0.6268	0.3726	1.9309	317.276	33.57	12.63
98-Int0	-8.8535	2.3119	-0.6277	0.3847	0.4208	249.789	35.99	12.96
99-Int0	-9.2764	2.1818	-0.6376	0.4067	3.6425	261.822	35.56	12.42
100-Int0	-9.0728	2.3524	-0.6368	0.3915	5.785	219.9413	35.19	11.23
101-Int0	-9.195	2.1821	-0.6302	0.4343	3.8484	222.613	35.99	12.17
102-Int0	-9.0913	2.4439	-0.6361	0.4004	3.9246	230.8473	36.65	13.05
103-Int0	-9.3419	2.3647	-0.6399	0.4041	4.851	219.9167	33.42	12.61
104-Int0	-9.2505	2.2781	-0.6345	0.3906	4.5747	215.3887	35.42	12.02
105-Int0	-9.1713	2.3277	-0.627	0.3684	4.39	229.478	34.48	13.35
106-Int0	-8.7095	2.1238	-0.6042	0.3774	5.5893	238.3157	36.45	11.24
107-Int0	-9.0636	2.0686	-0.638	0.4067	3.2301	289.087	34.82	10.88
108-Int0	-8.8391	2.1369	-0.6386	0.3953	5.1498	275.8737	33.21	9.41
109-Int0	-8.9904	2.11	-0.6294	0.426	3.2609	278.789	35.45	11.95
110-Int0	-9.2818	2.2354	-0.6283	0.3692	5.8638	286.6193	35.12	13.26
111-Int0	-9.4165	2.1456	-0.6284	0.369	4.7487	234.367	33.05	11.69
112-Int0	-8.9808	2.4444	-0.6354	0.3979	3.7395	234.287	36.36	13.24
113-Int0	-8.8954	2.2765	-0.6294	0.4087	2.9064	233.0173	36.1	13.83
114-Int0	-9.0192	2.1369	-0.6246	0.3897	4.8466	269.49	33.5	12.63
115-Int0	-8.8364	1.4327	-0.4122	0.1792	4.6971	284.3657	26.33	8.2
116-Int0	-9.1463	1.3978	-0.4105	0.1759	2.5031	217.374	26.53	5.77
117-Int0	-8.9017	1.4134	-0.4133	0.1888	1.6554	230.9443	26.2	5.82
118-Int0	-9.2862	1.3954	-0.4388	0.1721	3.0031	187.5823	26.57	5.7
119-Int0	-9.1191	1.4517	-0.4309	0.1832	5.1153	190.65	25.9	5.58
120-Int0	-9.257	1.5015	-0.425	0.1946	3.4622	198.6917	27.51	6.97
121-Int0	-9.0511	1.4566	-0.4202	0.1816	3.6547	188.6567	26.81	7.21
122-Int0	-9.3349	1.4732	-0.432	0.1825	5.0292	184.2317	27.02	6.62
123-Int0	-9.2364	1.483	-0.4281	0.1883	4.8367	197.6547	25.53	5.86
124-Int0	-9.1354	1.5263	-0.4185	0.1972	4.3505	206.205	25.97	6.64
125-Int0	-8.7378	1.3279	-0.3954	0.176	5.1377	255.664	23.9	3.1
126-Int0	-9.072	1.3315	-0.4338	0.1717	3.3068	242.2143	26.99	5.33
127-Int0	-8.8793	1.35	-0.4265	0.1926	5.626	246.1663	25.18	4.21
128-Int0	-9.0276	1.4215	-0.4199	0.1952	3.5007	253.6297	27.21	6.4

129-Int0	-9.2859	1.5312	-0.4138	0.1984	6.0934	202.1443	26.16	6.96
130-Int0	-9.4149	1.4773	-0.4224	0.1951	4.9902	202.5033	26.19	6.26
131-Int0	-8.9351	1.4438	-0.4193	0.1861	3.4207	202.2467	26.72	7.37
132-Int0	-8.8921	1.353	-0.4141	0.1859	2.6601	238.288	27.43	8.48
133-Int0	-9.0617	1.3919	-0.4204	0.1954	4.9179	245.483	25.41	5.63
134-Int0	-9.0845	2.2082	-0.4436	0.1958	4.4264	287.5023	29.99	9.81
135-Int0	-9.3776	2.1293	-0.4456	0.1745	2.0186	293.6837	31.3	11.06
136-Int0	-9.0516	2.0697	-0.4475	0.2043	1.474	226.475	30.08	8.76
137-Int0	-9.503	2.107	-0.4619	0.2064	4.0318	239.3097	31.43	9.27
138-Int0	-9.3218	2.178	-0.4607	0.2128	5.553	197.6037	29.95	7.54
139-Int0	-9.4674	2.1693	-0.4546	0.2415	3.7435	199.7057	30.59	8.73
140-Int0	-9.3164	2.2278	-0.4521	0.2135	4.0914	207.2857	30.97	9.45
141-Int0	-9.5719	2.2063	-0.462	0.2081	5.483	198.1043	32.26	9.06
142-Int0	-9.5292	2.2243	-0.4583	0.2122	4.8461	193.5547	31.94	8.63
143-Int0	-9.3686	2.224	-0.4485	0.2009	4.7154	206.204	29.84	8.77
144-Int0	-8.7378	1.3279	-0.3954	0.176	5.1376	215.409	23.9	3.1
145-Int0	-9.2736	1.9823	-0.4592	0.209	3.5168	255.6637	29.61	8.21
146-Int0	-8.9828	1.9298	-0.4547	0.2106	5.9327	251.5923	28.27	6.56
147-Int0	-9.1849	2.0224	-0.4494	0.2425	3.6566	256.8627	29.51	8.37
148-Int0	-9.4973	2.1647	-0.4499	0.2088	6.0311	262.8563	30.54	8.14
149-Int0	-9.6677	2.1638	-0.4523	0.2038	5.3553	209.9123	30.64	7.06
150-Int0	-9.2187	2.233	-0.4512	0.2134	3.1288	209.8053	30.13	9.4
151-Int0	-9.0886	2.0327	-0.4465	0.2184	2.7035	210.433	30.76	10.54
152-Int0	-9.2483	2.0474	-0.4516	0.209	5.2939	246.1227	30.82	8.75
153-Int0	-9.0908	2.5625	-0.4694	0.4136	3.6497	288.0957	31.47	11.39
154-Int0	-9.3365	2.3184	-0.4741	0.4046	2.0815	292.9907	31.03	10.83
155-Int0	-9.0592	2.4341	-0.4754	0.4171	0.4185	226.4407	33.39	11.04
156-Int0	-9.4976	2.3168	-0.4892	0.4449	3.8598	238.088	31.19	9.83
157-Int0	-9.3292	2.5119	-0.4858	0.4296	5.5379	197.9243	34.2	9.35
158-Int0	-9.4603	2.3639	-0.4783	0.4709	3.6785	199.6187	32.34	9.98
159-Int0	-9.3101	2.5709	-0.4802	0.4394	4.1979	207.5817	33.22	9.96
160-Int0	-9.5738	2.4983	-0.4904	0.4398	5.0983	197.5463	30.84	9.59
161-Int0	-9.4437	2.3897	-0.4846	0.4203	4.8352	193.009	31.37	9.81
162-Int0	-9.3455	2.4278	-0.4728	0.3998	4.6668	206.9513	32.77	9.96

163-Int0	-8.8813	2.2039	-0.4567	0.4134	5.4385	215.479	32.1	6.89
164-Int0	-9.275	2.2068	-0.4845	0.4455	3.4627	264.395	30.67	7.69
165-Int0	-9.0353	2.2629	-0.4821	0.42	5.4672	254.2203	32.31	6.82
166-Int0	-9.2105	2.2531	-0.4731	0.4683	3.1376	256.8783	31.22	8.86
167-Int0	-9.4881	2.3464	-0.4716	0.4104	5.8208	263.4887	31.8	9.38
168-Int0	-9.6315	2.2673	-0.4744	0.4077	4.7574	210.117	30.03	7.73
169-Int0	-9.2255	2.5992	-0.478	0.4413	3.4311	210.154	33.66	9.59
170-Int0	-9.0502	2.3639	-0.4753	0.4285	3.0772	209.838	34.09	12.38
171-Int0	-9.2317	2.2683	-0.4788	0.4215	4.8247	246.2757	30.53	9.8
172-Int0	-8.6968	1.3976	-0.5557	0.212	4.2231	299.5077	30.19	10.81
173-Int0	-8.9863	1.3388	-0.5542	0.1945	2.5711	228.767	25.59	6.06
174-Int0	-8.7629	1.3802	-0.5582	0.2182	1.4643	244.52	29.07	8.37
175-Int0	-9.1558	1.3957	-0.5844	0.1981	3.1542	200.877	28.21	7.66
176-Int0	-8.943	1.4294	-0.5772	0.2172	5.6075	203.4377	26.95	6.94
177-Int0	-9.0946	1.4504	-0.5738	0.2243	3.414	211.5087	27.74	7.81
178-Int0	-8.921	1.4289	-0.5695	0.203	3.6057	201.6117	27.71	8.41
179-Int0	-9.1632	1.433	-0.5662	0.209	4.9221	197.5943	27.54	8.06
180-Int0	-9.1	1.4509	-0.5717	0.2128	4.6524	210.6237	27.39	8
181-Int0	-8.9857	1.501	-0.5559	0.2237	4.2703	219.6287	27.28	7.94
182-Int0	-8.5808	1.2893	-0.5382	0.1991	5.0241	270.1167	24.8	4.21
183-Int0	-8.9381	1.3181	-0.5832	0.1986	3.2078	255.5227	25.46	4.67
184-Int0	-8.7297	1.3268	-0.5683	0.2219	5.3795	258.925	26.55	6.15
185-Int0	-8.8815	1.3744	-0.5721	0.2231	3.2752	266.4957	26.86	6.45
186-Int0	-9.0842	1.4357	-0.5596	0.2416	5.3378	216.7433	27.18	8.08
187-Int0	-9.2189	1.4316	-0.5646	0.238	4.7888	216.9847	25.62	5.95
188-Int0	-8.8059	1.4242	-0.5683	0.2046	3.3473	214.4057	28	8.52
189-Int0	-8.7719	1.3241	-0.5619	0.2101	2.5556	251.9767	28.94	9.58
190-Int0	-8.9406	1.3657	-0.5639	0.2193	4.7088	258.9517	26.2	6.64
191-Int0	-8.8905	2.0768	-0.5981	0.2154	4.3966	300.5627	30.15	10.1
192-Int0	-9.1509	1.9358	-0.5965	0.2185	2.6308	307.3613	28.75	8.71
193-Int0	-8.8807	1.9717	-0.5962	0.2162	1.3348	239.6287	31.28	11.49
194-Int0	-9.2383	1.9124	-0.6051	0.2125	3.8932	252.0203	31.5	9.96
195-Int0	-9.0214	1.996	-0.5994	0.2221	6.0284	210.3337	31.34	9.57
196-Int0	-9.2317	2.0077	-0.6053	0.2623	3.707	213.6537	30.77	8.65

197-Int0	-9.0393	2.0264	-0.6007	0.2115	3.9401	220.382	31.9	10.62
198-Int0	-9.2881	2.0199	-0.6018	0.2157	5.273	211.1303	31.14	10.12
199-Int0	-9.2736	2.0528	-0.6066	0.2286	4.8298	206.895	29.62	9.63
200-Int0	-9.1512	2.0939	-0.5933	0.2159	4.5925	219.584	30.39	10.02
201-Int0	-8.5808	1.2893	-0.5382	0.1991	5.0241	228.8147	24.8	4.21
202-Int0	-9.023	1.8183	-0.6056	0.2119	3.6871	270.1167	30.87	9.15
203-Int0	-8.7928	1.8289	-0.601	0.2232	5.661	266.3663	30.35	8.41
204-Int0	-8.9939	1.8977	-0.6055	0.2635	3.4774	269.5147	30.22	8.41
205-Int0	-9.2813	2.0634	-0.5946	0.214	6.2367	276.0043	30.49	9.41
206-Int0	-9.4214	2.0278	-0.5941	0.2099	5.3283	224.574	30.43	8.82
207-Int0	-8.9226	2.0215	-0.6004	0.2129	3.6757	224.4427	31.18	10.54
208-Int0	-8.8766	1.9157	-0.5947	0.2188	3.0402	224.31	32.42	11.91
209-Int0	-9.0437	1.92	-0.591	0.2283	5.0646	261.5307	30.7	10.55
210-Int0	-8.8989	2.4205	-0.6323	0.3981	3.1376	300.2303	32.43	11.16
211-Int0	-9.1408	2.1726	-0.6277	0.3865	5.8208	306.402	32.43	11.51
212-Int0	-8.8959	2.3203	-0.6335	0.3922	4.7574	239.68	34.88	12.26
213-Int0	-9.2399	2.1154	-0.6398	0.4099	3.4311	250.905	32.3	11.42
214-Int0	-9.1087	2.3535	-0.6419	0.4227	3.0772	210.293	34.16	9.87
215-Int0	-9.247	2.2049	-0.6354	0.4639	4.8247	212.3093	31.57	9.79
216-Int0	-9.0508	2.3693	-0.6385	0.4006	5.5908	220.336	36.11	12.22
217-Int0	-9.2919	2.2942	-0.6371	0.4101	3.6399	210.1117	32.31	10.94
218-Int0	-9.2878	2.2917	-0.6395	0.4151	6.2889	205.791	31.91	10.44
219-Int0	-9.1441	2.2931	-0.6243	0.3746	5.0199	218.9693	33.52	11.09
220-Int0	-8.718	2.1149	-0.6073	0.4087	4.2729	228.4813	33.01	8.48
221-Int0	-9.0228	2.0038	-0.6398	0.4081	3.4839	278.424	30.84	10.29
222-Int0	-8.8274	2.1059	-0.6394	0.3885	4.9464	267.074	32.4	8.14
223-Int0	-9.0189	2.1094	-0.6345	0.4598	3.9552	269.58	31.22	8.91
224-Int0	-9.2916	2.2177	-0.6278	0.4044	6.6064	276.3347	32.87	10.22
225-Int0	-9.4293	2.1307	-0.6276	0.4024	5.5833	224.297	31.74	9.27
226-Int0	-9.0097	2.4409	-0.6405	0.4285	4.2222	224.22	34.62	11.14
227-Int0	-8.8867	2.2504	-0.6326	0.3997	3.4641	222.6233	35.91	13.47
228-Int0	-9.0355	2.1323	-0.6256	0.4039	5.3304	259.9797	32.24	10.84

Table S6. The DFT calculated energies of all optimized structures in the machine learning sample dataset

Species	Gc hatree	G(gas) hatree	Esp + Sol hatree	Final G hartree
1-Int0	0.491103	-2737.110193	-2739.450647	-2738.959544
1-TS3	0.590512	-2931.185403	-2933.835816	-2933.245304
1-Int2	0.510735	-2738.276528	-2740.631949	-2740.121214
2-Int0	0.492112	-1564.356665	-1566.547814	-1566.055702
2-TS3	0.591696	-1758.423825	-1760.919606	-1760.327910
2-Int2	0.509683	-1565.516593	-1567.722692	-1567.213009
3-Int0	0.491924	-1568.564024	-1570.767073	-1570.275149
3-TS3	0.587480	-1762.638574	-1765.147181	-1764.559701
3-Int2	0.510231	-1569.727694	-1571.944862	-1571.434631
4-Int0	0.363827	-2407.616593	-2409.476314	-2409.112487
4-TS3	0.464011	-2601.692222	-2603.863710	-2603.399699
4-Int2	0.383377	-2408.782882	-2410.663557	-2410.280180
5-Int0	0.362641	-1234.865743	-1236.574610	-1236.211969
5-TS3	0.455512	-1428.938246	-1430.948606	-1430.493094
5-Int2	0.381857	-1236.023803	-1237.752783	-1237.370926
6-Int0	0.362358	-1239.074520	-1240.795273	-1240.432915
6-TS3	0.458318	-1433.148022	-1435.175256	-1434.716938
6-Int2	0.382306	-1240.235895	-1241.975584	-1241.593278
7-Int0	0.350245	-2500.570090	-2502.186844	-2501.836599
7-TS3	0.447973	-2694.644662	-2696.573933	-2696.125960
7-Int2	0.370528	-2501.736373	-2503.372850	-2503.002322
8-Int0	0.348269	-1327.820052	-1329.285806	-1328.937537
8-TS3	0.444752	-1521.887098	-1523.659373	-1523.214621
8-Int2	0.367861	-1328.979123	-1330.463289	-1330.095428
9-Int0	0.348327	-1332.026971	-1333.504752	-1333.156425
9-TS3	0.445689	-1526.097934	-1527.885387	-1527.439698
9-Int2	0.368627	-1333.189985	-1334.685203	-1334.316576
10-Int0	0.323344	-2183.833989	-2185.404307	-2185.080963
10-TS3	0.421825	-2377.907805	-2379.790600	-2379.368775
10-Int2	0.345190	-2185.000317	-2186.590537	-2186.245347
11-Int0	0.337721	-2164.013311	-2165.574480	-2165.236759
11-TS3	0.436535	-2358.086666	-2359.961362	-2359.524827
11-Int2	0.358227	-2165.183284	-2166.760972	-2166.402745
12-Int0	0.321234	-2506.796008	-2508.412250	-2508.091016
12-TS3	0.418428	-2700.869197	-2702.796225	-2702.377797
12-Int2	0.341506	-2507.962513	-2509.596568	-2509.255062
13-Int0	0.337587	-2164.044544	-2165.601598	-2165.264011
13-TS3	0.436181	-2358.116508	-2359.986687	-2359.550506
13-Int2	0.358454	-2165.208190	-2166.784581	-2166.426127
14-Int0	0.324031	-2183.870377	-2185.442911	-2185.118880
14-TS3	0.422651	-2377.943395	-2379.828183	-2379.405532
14-Int2	0.345500	-2185.035163	-2186.626851	-2186.281351
15-Int0	0.320807	-2506.802498	-2508.417210	-2508.096403
15-TS3	0.418550	-2700.876391	-2702.802971	-2702.384421
15-Int2	0.341689	-2507.968554	-2509.601528	-2509.259839
16-Int0	0.354677	-2186.067867	-2187.660863	-2187.306186

16-TS3	0.453736	-2380.140175	-2382.046766	-2381.593030
16-Int2	0.375484	-2187.234754	-2188.845274	-2188.469790
17-Int0	0.401881	-2414.693011	-2416.579388	-2416.177507
17-TS3	0.502379	-2608.766503	-2610.963522	-2610.461143
17-Int2	0.423154	-2415.865695	-2417.766562	-2417.343408
18-Int0	0.367922	-2337.317175	-2339.086919	-2338.718997
18-TS3	0.465441	-2531.391991	-2533.473597	-2533.008156
18-Int2	0.389494	-2338.483918	-2340.274308	-2339.884814
19-Int0	0.380573	-2317.492298	-2319.251307	-2318.870734
19-TS3	0.479642	-2511.566020	-2513.638932	-2513.159290
19-Int2	0.402334	-2318.661976	-2320.439727	-2320.037393
20-Int0	0.365051	-2660.279572	-2662.092908	-2661.727857
20-TS3	0.462280	-2854.352505	-2856.477439	-2856.015159
20-Int2	0.385758	-2661.445505	-2663.278143	-2662.892385
21-Int0	0.341777	-2202.091458	-2203.700461	-2203.358684
21-TS3	0.439909	-2396.165660	-2398.085247	-2397.645338
21-Int2	0.362856	-2203.260015	-2204.884536	-2204.521680
22-Int0	0.362997	-2203.297564	-2204.917937	-2204.554940
22-TS3	0.461990	-2397.369144	-2399.303135	-2398.841145
22-Int2	0.383384	-2204.461602	-2206.101034	-2205.717650
23-Int0	0.342167	-2202.087159	-2203.692974	-2203.350807
23-TS3	0.440513	-2396.160720	-2398.078291	-2397.637778
23-Int2	0.364402	-2203.253839	-2204.878472	-2204.514070
24-Int0	0.382113	-2317.524818	-2319.283890	-2318.901777
24-TS3	0.480753	-2511.597957	-2513.668576	-2513.187823
24-Int2	0.402313	-2318.689699	-2320.466209	-2320.063896
25-Int0	0.365035	-2660.282631	-2662.097067	-2661.732032
25-TS3	0.463723	-2854.359397	-2856.486022	-2856.022299
25-Int2	0.385840	-2661.453107	-2663.285531	-2662.899691
26-Int0	0.322998	-1011.078454	-1012.500269	-1012.177271
26-TS3	0.417845	-1205.148343	-1206.873779	-1206.455934
26-Int2	0.343308	-1012.240425	-1013.678900	-1013.335592
27-Int0	0.323310	-1015.285748	-1016.719549	-1016.396239
27-TS3	0.419744	-1209.358444	-1211.099304	-1210.679560
27-Int2	0.344360	-1016.451321	-1017.900841	-1017.556481
28-Int0	0.337005	-991.259713	-992.670824	-992.333819
28-TS3	0.432208	-1185.328421	-1187.045632	-1186.613424
28-Int2	0.356774	-992.424605	-993.850273	-993.493499
29-Int0	0.337235	-995.466440	-996.889403	-996.552168
29-TS3	0.431935	-1189.540394	-1191.270740	-1190.838805
29-Int2	0.357394	-996.635403	-998.071783	-997.714389
30-Int0	0.317257	-1334.044575	-1335.507734	-1335.190477
30-TS3	0.415295	-1528.110536	-1529.880638	-1529.465343
30-Int2	0.338872	-1335.204690	-1336.685621	-1336.346749
31-Int0	0.317870	-1338.251321	-1339.727417	-1339.409547
31-TS3	0.415124	-1532.322345	-1534.105970	-1533.690846
31-Int2	0.339548	-1339.415500	-1340.907600	-1340.568052
32-Int0	0.336720	-991.290823	-992.698362	-992.361642
32-TS3	0.431839	-1185.358582	-1187.071061	-1186.639222
32-Int2	0.356050	-992.450609	-993.874707	-993.518657
33-Int0	0.337186	-995.497442	-996.917082	-996.579897
33-TS3	0.433156	-1189.569189	-1191.296381	-1190.863225
33-Int2	0.356538	-996.661743	-998.095874	-997.739336
34-Int0	0.323974	-1011.114555	-1012.538356	-1012.214382
34-TS3	0.418903	-1205.184503	-1206.911468	-1206.492565
34-Int2	0.342574	-1012.277700	-1013.715852	-1013.373278
35-Int0	0.324105	-1015.322471	-1016.758346	-1016.434241
35-TS3	0.419864	-1209.395760	-1211.137903	-1210.718039
35-Int2	0.344918	-1016.487326	-1017.938026	-1017.593108
36-Int0	0.319976	-1334.047813	-1335.512186	-1335.192210

36-TS3	0.414475	-1528.117844	-1529.886506	-1529.472031
36-Int2	0.338989	-1335.210445	-1336.690658	-1336.351669
37-Int0	0.320123	-1338.255276	-1339.731745	-1339.411622
37-TS3	0.415856	-1532.328446	-1534.112165	-1533.696309
37-Int2	0.339953	-1339.421195	-1340.912423	-1340.572470
38-Int0	0.352611	-1013.314905	-1014.757028	-1014.404417
38-TS3	0.448369	-1207.382821	-1209.130890	-1208.682521
38-Int2	0.373722	-1014.475242	-1015.934757	-1015.561035
39-Int0	0.352959	-1017.521692	-1018.975514	-1018.622555
39-TS3	0.448977	-1211.593874	-1213.356361	-1212.907384
39-Int2	0.372362	-1018.688018	-1020.156224	-1019.783862
40-Int0	0.399873	-1241.939781	-1243.674226	-1243.274353
40-TS3	0.499138	-1436.011546	-1438.049368	-1437.550230
40-Int2	0.420574	-1243.106708	-1244.855290	-1244.434716
41-Int0	0.399173	-1246.148805	-1247.895243	-1247.496070
41-TS3	0.501726	-1440.218309	-1442.276275	-1441.774549
41-Int2	0.420294	-1247.319366	-1249.078324	-1248.658030
42-Int0	0.366721	-1164.562621	-1166.182585	-1165.815864
42-TS3	0.462104	-1358.631706	-1360.557076	-1360.094972
42-Int2	0.386837	-1165.724874	-1167.362642	-1166.975805
43-Int0	0.367089	-1168.769476	-1170.401813	-1170.034724
43-TS3	0.463418	-1362.842222	-1364.782244	-1364.318826
43-Int2	0.387293	-1169.935900	-1171.584319	-1171.197026
44-Int0	0.361704	-1030.544361	-1032.013593	-1031.651889
44-TS3	0.457743	-1224.610979	-1226.390924	-1225.933181
44-Int2	0.381301	-1031.703727	-1033.194187	-1032.812886
45-Int0	0.380302	-1144.738251	-1146.347340	-1145.967038
45-TS3	0.475319	-1338.807598	-1340.723414	-1340.248095
45-Int2	0.400480	-1145.903753	-1147.529195	-1147.128715
46-Int0	0.380657	-1148.944627	-1150.566299	-1150.185642
46-TS3	0.476186	-1343.018268	-1344.948588	-1344.472402
46-Int2	0.400879	-1150.114364	-1151.750619	-1151.349740
47-Int0	0.362204	-1487.527153	-1489.188404	-1488.826200
47-TS3	0.458762	-1681.594233	-1683.561656	-1683.102894
47-Int2	0.383641	-1488.687095	-1490.366997	-1489.983356
48-Int0	0.362552	-1491.733780	-1493.407499	-1493.044947
48-TS3	0.459283	-1685.805204	-1687.786863	-1687.327580
48-Int2	0.383163	-1492.898761	-1494.588665	-1494.205502
49-Int0	0.340333	-1029.336900	-1030.795567	-1030.455234
49-TS3	0.437011	-1223.405575	-1225.168993	-1224.731982
49-Int2	0.361090	-1030.500466	-1031.973614	-1031.612524
50-Int0	0.340837	-1033.544065	-1035.014798	-1034.673961
50-TS3	0.437499	-1227.617105	-1229.394889	-1228.957390
50-Int2	0.361675	-1034.711520	-1036.195640	-1035.833965
51-Int0	0.362709	-1034.750074	-1036.232649	-1035.869940
51-TS3	0.458486	-1228.822045	-1230.613085	-1230.154599
51-Int2	0.381465	-1035.914915	-1037.412556	-1037.031091
52-Int0	0.339794	-1029.333424	-1030.787869	-1030.448075
52-TS3	0.436113	-1223.402731	-1225.162395	-1224.726282
52-Int2	0.361136	-1030.495936	-1031.967676	-1031.606540
53-Int0	0.340639	-1033.540337	-1035.007128	-1034.666489
53-TS3	0.437154	-1227.613297	-1229.387600	-1228.950446
53-Int2	0.361172	-1034.707276	-1036.189195	-1035.828023
54-Int0	0.380797	-1144.773447	-1146.382312	-1146.001515
54-TS3	0.475389	-1338.841185	-1340.752937	-1340.277548
54-Int2	0.400490	-1145.931293	-1147.556154	-1147.155664
55-Int0	0.380765	-1148.980017	-1150.600799	-1150.220034
55-TS3	0.476825	-1343.051474	-1344.978673	-1344.501848
55-Int2	0.400681	-1150.142620	-1151.777841	-1151.377160
56-Int0	0.364288	-1487.530981	-1489.196065	-1488.831777

56-TS3	0.458910	-1681.602351	-1683.570608	-1683.111698
56-Int2	0.384190	-1488.694323	-1490.375397	-1489.991207
57-Int0	0.364100	-1491.738315	-1493.415500	-1493.051400
57-TS3	0.460304	-1685.812654	-1687.796457	-1687.336153
57-Int2	0.383897	-1492.906115	-1494.597131	-1494.213234
58-Int0	0.464414	-2697.859195	-2700.130899	-2699.666485
58-TS3	0.562823	-2891.928116	-2894.508220	-2893.945397
58-Int2	0.484352	-2699.017486	-2701.307222	-2700.822870
59-Int0	0.336465	-2368.366952	-2370.158571	-2369.822106
59-TS3	0.434355	-2562.438119	-2564.539155	-2564.104800
59-Int2	0.356288	-2369.525199	-2371.337743	-2370.981455
60-Int0	0.322539	-2461.320777	-2462.869095	-2462.546556
60-TS3	0.421591	-2655.388320	-2657.249108	-2656.827517
60-Int2	0.342019	-2462.480098	-2464.047068	-2463.705049
61-Int0	0.296678	-2144.582389	-2146.085189	-2145.788511
61-TS3	0.394927	-2338.651501	-2340.465410	-2340.070483
61-Int2	0.317097	-2145.744249	-2147.265144	-2146.948047
62-Int0	0.309842	-2124.763725	-2126.255750	-2125.945908
62-TS3	0.408532	-2318.831533	-2320.636752	-2320.228220
62-Int2	0.331098	-2125.926108	-2127.435635	-2127.104537
63-Int0	0.292699	-2467.546529	-2469.093434	-2468.800735
63-TS3	0.392057	-2661.612560	-2663.471129	-2663.079072
63-Int2	0.313624	-2468.706217	-2470.271108	-2469.957484
64-Int0	0.310674	-2124.793165	-2126.282410	-2125.971736
64-TS3	0.408838	-2318.861235	-2320.661981	-2320.253143
64-Int2	0.331171	-2125.951835	-2127.459690	-2127.128519
65-Int0	0.297532	-2144.618518	-2146.123487	-2145.825955
65-TS3	0.395846	-2338.687547	-2340.503591	-2340.107745
65-Int2	0.318281	-2145.778609	-2147.301999	-2146.983718
66-Int0	0.292946	-2467.552051	-2469.098293	-2468.805347
66-TS3	0.391724	-2661.620240	-2663.478116	-2663.086392
66-Int2	0.313527	-2468.712277	-2470.276199	-2469.962672
67-Int0	0.326818	-2146.817989	-2148.342549	-2148.015731
67-TS3	0.424987	-2340.885521	-2342.721457	-2342.296470
67-Int2	0.348682	-2147.976498	-2149.519551	-2149.170869
68-Int0	0.375807	-2375.441163	-2377.258700	-2376.882893
68-TS3	0.473024	-2569.514110	-2571.639788	-2571.166764
68-Int2	0.396640	-2376.607401	-2378.440474	-2378.043834
69-Int0	0.340455	-2298.066202	-2299.767727	-2299.427272
69-TS3	0.439058	-2492.135219	-2494.148282	-2493.709224
69-Int2	0.361654	-2299.227753	-2300.948952	-2300.587298
70-Int0	0.353982	-2278.240877	-2279.932124	-2279.578142
70-TS3	0.451904	-2472.310553	-2474.314240	-2473.862336
70-Int2	0.374365	-2279.405814	-2281.114751	-2280.740386
71-Int0	0.337021	-2621.029460	-2622.773814	-2622.436793
71-TS3	0.435966	-2815.095836	-2817.152191	-2816.716225
71-Int2	0.357821	-2622.189311	-2623.952791	-2623.594970
72-Int0	0.315148	-2162.840493	-2164.382107	-2164.066959
72-TS3	0.412487	-2356.910052	-2358.759902	-2358.347415
72-Int2	0.335833	-2164.001753	-2165.558650	-2165.222817
73-Int0	0.315022	-2162.836330	-2164.374425	-2164.059403
73-TS3	0.412257	-2356.905746	-2358.752568	-2358.340311
73-Int2	0.335527	-2163.997669	-2165.552854	-2165.217327
74-Int0	0.335635	-2164.046763	-2165.598736	-2165.263101
74-TS3	0.434924	-2358.113613	-2359.978673	-2359.543749
74-Int2	0.356875	-2165.204479	-2166.775977	-2166.419102
75-Int0	0.355381	-2278.273630	-2279.965214	-2279.609833
75-TS3	0.451982	-2472.343161	-2474.343008	-2473.891026
75-Int2	0.375631	-2279.431722	-2281.140751	-2280.765120
76-Int0	0.339072	-2621.031429	-2622.779485	-2622.440413

76-TS3	0.436040	-2815.103902	-2817.160857	-2816.724817
76-Int2	0.359501	-2622.194471	-2623.959545	-2623.600044
77-Int0	0.463894	-1529.312781	-1531.445932	-1530.982038
77-TS3	0.560317	-1723.380843	-1725.818545	-1725.258228
77-Int2	0.484158	-1530.469555	-1532.618278	-1532.134120
78-Int0	0.336193	-1199.821534	-1201.475804	-1201.139611
78-TS3	0.429647	-1393.892302	-1395.848861	-1395.419214
78-Int2	0.355457	-1200.977332	-1202.648874	-1202.293417
79-Int0	0.322081	-1292.773812	-1294.184412	-1293.862331
79-TS3	0.418078	-1486.841944	-1488.558744	-1488.140666
79-Int2	0.340759	-1293.932590	-1295.358361	-1295.017602
80-Int0	0.294776	-976.033756	-977.397576	-977.102800
80-TS3	0.391374	-1170.102632	-1171.772025	-1171.380651
80-Int2	0.317407	-977.193174	-978.574407	-978.257000
81-Int0	0.310485	-956.213396	-957.567976	-957.257491
81-TS3	0.405781	-1150.282759	-1151.944058	-1151.538277
81-Int2	0.329722	-957.378123	-958.745602	-958.415880
82-Int0	0.292321	-1298.996799	-1300.405644	-1300.113323
82-TS3	0.388868	-1493.064630	-1494.779408	-1494.390540
82-Int2	0.311339	-1300.158665	-1301.580858	-1301.269519
83-Int0	0.310008	-956.244345	-957.594857	-957.284849
83-TS3	0.405945	-1150.312523	-1151.969829	-1151.563884
83-Int2	0.329852	-957.403875	-958.769987	-958.440135
84-Int0	0.296590	-976.069677	-977.435973	-977.139383
84-TS3	0.392964	-1170.138770	-1171.810753	-1171.417789
84-Int2	0.316985	-977.230525	-978.611652	-978.294667
85-Int0	0.292060	-1299.002968	-1300.410572	-1300.118512
85-TS3	0.388245	-1493.072022	-1494.785789	-1494.397544
85-Int2	0.311850	-1300.164240	-1301.585587	-1301.273737
86-Int0	0.325920	-978.268642	-979.654225	-979.328305
86-TS3	0.422491	-1172.336142	-1174.029283	-1173.606792
86-Int2	0.347016	-979.427800	-980.829368	-980.482352
87-Int0	0.375807	-2375.441163	-2377.258700	-2376.882893
87-TS3	0.473024	-2569.514110	-2571.639788	-2571.166764
87-Int2	0.396640	-2376.607401	-2378.440474	-2378.043834
88-Int0	0.338816	-1129.517048	-1131.080008	-1130.741192
88-TS3	0.435942	-1323.585501	-1325.455242	-1325.019300
88-Int2	0.360982	-1130.677285	-1132.257694	-1131.896712
89-Int0	0.353050	-1109.692303	-1111.244907	-1110.891857
89-TS3	0.449285	-1303.761438	-1305.621801	-1305.172516
89-Int2	0.373440	-1110.857161	-1112.424591	-1112.051151
90-Int0	0.335634	-1452.480505	-1454.086235	-1453.750601
90-TS3	0.432959	-1646.547552	-1648.460383	-1648.027424
90-Int2	0.357557	-1453.639489	-1455.262459	-1454.904902
91-Int0	0.315767	-994.289122	-995.693312	-995.377545
91-TS3	0.410204	-1188.359889	-1190.067353	-1189.657149
91-Int2	0.334531	-995.452974	-996.868423	-996.533892
92-Int0	0.313541	-994.287106	-995.685513	-995.371972
92-TS3	0.409741	-1188.356567	-1190.060558	-1189.650817
92-Int2	0.334760	-995.448111	-996.862438	-996.527678
93-Int0	0.335033	-995.497602	-996.911279	-996.576246
93-TS3	0.431852	-1189.564890	-1191.286892	-1190.855040
93-Int2	0.356048	-996.655907	-998.086350	-997.730302
94-Int0	0.353354	-1109.726975	-1111.279150	-1110.925796
94-TS3	0.448401	-1303.795938	-1305.652159	-1305.203758
94-Int2	0.373204	-1110.884867	-1112.451765	-1112.078561
95-Int0	0.337838	-1452.485088	-1454.094937	-1453.757099
95-TS3	0.433144	-1646.555470	-1648.469279	-1648.036135
95-Int2	0.356961	-1453.647440	-1455.270104	-1454.913143
96-Int0	0.463527	-1525.105495	-1527.225895	-1526.762368

96-TS3	0.559486	-1719.170087	-1721.593473	-1721.033987
96-Int2	0.483819	-1526.258212	-1528.396314	-1527.912495
97-Int0	0.335480	-1195.613331	-1197.254463	-1196.918983
97-TS3	0.428483	-1389.681636	-1391.623421	-1391.194938
97-Int2	0.354388	-1196.765684	-1198.425944	-1198.071556
98-Int0	0.321022	-1288.567576	-1289.964919	-1289.643897
98-TS3	0.416967	-1482.631788	-1484.332970	-1483.916003
98-Int2	0.340821	-1289.720912	-1291.136762	-1290.795941
99-Int0	0.294562	-971.825760	-973.178195	-972.883632
99-TS3	0.390827	-1165.892000	-1167.547250	-1167.156423
99-Int2	0.315898	-972.982703	-974.352443	-974.036545
100-Int0	0.308364	-952.007955	-953.349131	-953.040767
100-TS3	0.404638	-1146.072775	-1147.718783	-1147.314145
100-Int2	0.328571	-953.167936	-954.524136	-954.195565
101-Int0	0.291226	-1294.789975	-1296.185988	-1295.894762
101-TS3	0.387280	-1488.855224	-1490.554149	-1490.166869
101-Int2	0.311093	-1295.947341	-1297.359159	-1297.048066
102-Int0	0.308858	-952.037843	-953.376047	-953.067189
102-TS3	0.404974	-1146.102074	-1147.743204	-1147.338230
102-Int2	0.329598	-953.192561	-954.548689	-954.219091
103-Int0	0.294614	-971.862976	-973.215835	-972.921221
103-TS3	0.391045	-1165.929942	-1167.588455	-1167.197410
103-Int2	0.315941	-973.019550	-974.389773	-974.073832
104-Int0	0.291475	-1294.795312	-1296.190392	-1295.898917
104-TS3	0.387827	-1488.861284	-1490.559750	-1490.171923
104-Int2	0.311865	-1295.952580	-1297.364321	-1297.052456
105-Int0	0.325030	-974.061738	-975.434875	-975.109845
105-TS3	0.419368	-1168.128150	-1169.803718	-1169.384350
105-Int2	0.346730	-975.216492	-976.607998	-976.261268
106-Int0	0.373587	-1202.687095	-1204.356672	-1203.983085
106-TS3	0.470080	-1396.755259	-1398.724540	-1398.254460
106-Int2	0.393738	-1203.847849	-1205.531604	-1205.137866
107-Int0	0.338603	-1125.309490	-1126.860125	-1126.521522
107-TS3	0.435169	-1319.375116	-1321.230650	-1320.795481
107-Int2	0.359377	-1126.467352	-1128.036258	-1127.676881
108-Int0	0.351624	-1105.486386	-1107.025364	-1106.673740
108-TS3	0.446616	-1299.553032	-1301.396879	-1300.950263
108-Int2	0.372086	-1106.647653	-1108.203526	-1107.831440
109-Int0	0.335584	-1448.273098	-1449.866491	-1449.530907
109-TS3	0.431651	-1642.337966	-1644.235516	-1643.803865
109-Int2	0.356316	-1449.429462	-1451.040886	-1450.684570
110-Int0	0.312649	-990.083891	-991.473505	-991.160856
110-TS3	0.408427	-1184.150322	-1185.842769	-1185.434342
110-Int2	0.334394	-991.241320	-992.646812	-992.312418
111-Int0	0.312735	-990.079435	-991.465608	-991.152873
111-TS3	0.410105	-1184.146254	-1185.839760	-1185.429655
111-Int2	0.334199	-991.237156	-992.641138	-992.306939
112-Int0	0.334189	-991.291171	-992.692491	-992.358302
112-TS3	0.430770	-1185.354448	-1187.060578	-1186.629808
112-Int2	0.355213	-992.445461	-993.865119	-993.509906
113-Int0	0.353649	-1105.519619	-1107.059684	-1106.706035
113-TS3	0.448137	-1299.584981	-1301.426104	-1300.977967
113-Int2	0.373000	-1106.673697	-1108.229701	-1107.856701
114-Int0	0.337023	-1448.278407	-1449.875420	-1449.538397
114-TS3	0.430604	-1642.347198	-1644.245062	-1643.814458
114-Int2	0.357234	-1449.435547	-1451.048205	-1450.690971
115-Int0	0.412661	-2619.354221	-2621.492594	-2621.079933
115-TS3	0.508390	-2813.431043	-2815.875818	-2815.367428
115-Int2	0.431901	-2620.514449	-2622.671465	-2622.239564
116-Int0	0.283294	-2289.863374	-2291.519805	-2291.236511

116-TS3	0.380674	-2483.938569	-2485.904363	-2485.523689
116-Int2	0.301886	-2291.022891	-2292.701899	-2292.400013
117-Int0	0.270046	-2382.816128	-2384.229873	-2383.959827
117-TS3	0.367270	-2576.889444	-2578.614805	-2578.247535
117-Int2	0.288796	-2383.977609	-2385.412054	-2385.123258
118-Int0	0.244088	-2066.075823	-2067.444614	-2067.200526
118-TS3	0.341128	-2260.150273	-2261.828764	-2261.487636
118-Int2	0.263867	-2067.240100	-2068.628006	-2068.364139
119-Int0	0.257394	-2046.257368	-2047.615613	-2047.358219
119-TS3	0.354503	-2240.331628	-2242.000909	-2241.646406
119-Int2	0.277739	-2047.423871	-2048.799765	-2048.522026
120-Int0	0.240503	-2389.039722	-2390.453311	-2390.212808
120-TS3	0.336850	-2583.113191	-2584.835267	-2584.498417
120-Int2	0.260403	-2390.202738	-2391.634798	-2391.374395
121-Int0	0.257809	-2046.287463	-2047.641901	-2047.384092
121-TS3	0.354946	-2240.360414	-2242.025768	-2241.670822
121-Int2	0.277711	-2047.448171	-2048.823017	-2048.545306
122-Int0	0.244623	-2066.112534	-2067.482883	-2067.238260
122-TS3	0.342253	-2260.186307	-2261.866903	-2261.524650
122-Int2	0.264343	-2067.275209	-2068.664755	-2068.400412
123-Int0	0.240989	-2389.045423	-2390.457218	-2390.216229
123-TS3	0.336823	-2583.120647	-2584.841816	-2584.504993
123-Int2	0.259914	-2390.209189	-2391.639501	-2391.379587
124-Int0	0.274944	-2068.312040	-2069.702409	-2069.427465
124-TS3	0.371614	-2262.385907	-2264.087154	-2263.715540
124-Int2	0.294726	-2069.475499	-2070.884307	-2070.589581
125-Int0	0.322492	-2296.936012	-2298.618940	-2298.296448
125-TS3	0.420026	-2491.016980	-2493.007844	-2492.587818
125-Int2	0.343536	-2298.107852	-2299.807749	-2299.464213
126-Int0	0.286943	-2219.560666	-2221.127273	-2220.840330
126-TS3	0.384903	-2413.634275	-2415.511675	-2415.126772
126-Int2	0.307371	-2220.724992	-2222.311908	-2222.004537
127-Int0	0.301033	-2199.735700	-2201.292582	-2200.991549
127-TS3	0.397732	-2393.810726	-2395.678601	-2395.280869
127-Int2	0.321551	-2200.903334	-2202.479095	-2202.157544
128-Int0	0.284064	-2542.523679	-2544.133540	-2543.849476
128-TS3	0.380900	-2736.596393	-2738.516471	-2738.135571
128-Int2	0.304596	-2543.686125	-2545.316564	-2545.011968
129-Int0	0.262554	-2084.334783	-2085.741584	-2085.479030
129-TS3	0.358797	-2278.411079	-2280.125600	-2279.766803
129-Int2	0.282668	-2085.500722	-2086.923306	-2086.640638
130-Int0	0.261866	-2084.330270	-2085.733957	-2085.472091
130-TS3	0.358376	-2278.406223	-2280.118188	-2279.759812
130-Int2	0.282421	-2085.495335	-2086.917243	-2086.634822
131-Int0	0.282628	-2085.541688	-2086.957704	-2086.675076
131-TS3	0.379742	-2279.614375	-2281.341684	-2280.961942
131-Int2	0.303597	-2086.701079	-2088.139627	-2087.836030
132-Int0	0.302032	-2199.769132	-2201.325447	-2201.023415
132-TS3	0.398657	-2393.842610	-2395.707813	-2395.309156
132-Int2	0.321909	-2200.928852	-2202.504513	-2202.182604
133-Int0	0.285810	-2542.526996	-2544.140007	-2543.854197
133-TS3	0.381751	-2736.604554	-2738.524913	-2738.143162
133-Int2	0.305879	-2543.692424	-2545.323803	-2545.017924
134-Int0	0.411599	-1450.808011	-1452.805669	-1452.394070
134-TS3	0.506934	-1644.880152	-1647.182668	-1646.675734
134-Int2	0.430448	-1451.966864	-1453.981587	-1453.551139
135-Int0	0.281749	-1121.318524	-1122.836678	-1122.554929
135-TS3	0.377310	-1315.390273	-1317.211812	-1316.834502
135-Int2	0.301138	-1122.474224	-1124.011139	-1123.710001
136-Int0	0.267368	-1214.270812	-1215.543491	-1215.276123

136-TS3	0.363583	-1408.341502	-1409.921230	-1409.557647
136-Int2	0.286706	-1215.430273	-1216.721570	-1216.434864
137-Int0	0.242870	-897.527727	-898.757668	-898.514798
137-TS3	0.337874	-1091.600283	-1093.132035	-1092.794161
137-Int2	0.263218	-898.689418	-899.935950	-899.672733
138-Int0	0.256055	-877.709474	-878.927768	-878.671713
138-TS3	0.351749	-1071.781486	-1073.305191	-1072.953442
138-Int2	0.276046	-878.875342	-880.108428	-879.832382
139-Int0	0.239425	-1220.491233	-1221.765572	-1221.526147
139-TS3	0.333797	-1414.564026	-1416.140657	-1415.806860
139-Int2	0.258216	-1221.654483	-1222.943156	-1222.684940
140-Int0	0.256471	-877.739806	-878.954954	-878.698483
140-TS3	0.351771	-1071.810762	-1073.330346	-1072.978575
140-Int2	0.275586	-878.900556	-880.131715	-879.856129
141-Int0	0.243594	-897.564292	-898.795881	-898.552287
141-TS3	0.339378	-1091.636898	-1093.169708	-1092.830330
141-Int2	0.262388	-898.727195	-899.972941	-899.710553
142-Int0	0.239372	-1220.496981	-1221.769883	-1221.530511
142-TS3	0.335197	-1414.569571	-1416.144269	-1415.809072
142-Int2	0.258758	-1221.660007	-1222.948211	-1222.689453
143-Int0	0.272702	-899.763578	-901.014033	-900.741331
143-TS3	0.367945	-1093.835710	-1095.391172	-1095.023227
143-Int2	0.292667	-900.926016	-902.192720	-901.900053
144-Int0	0.322492	-2296.936013	-2298.618940	-2298.296448
144-TS3	0.420026	-2491.016980	-2493.007844	-2492.587818
144-Int2	0.343536	-2298.107852	-2299.807749	-2299.464213
145-Int0	0.287038	-1051.010543	-1052.439409	-1052.152371
145-TS3	0.381898	-1245.083576	-1246.816542	-1246.434644
145-Int2	0.306946	-1052.173706	-1053.618930	-1053.311984
146-Int0	0.299644	-1031.187864	-1032.604864	-1032.305220
146-TS3	0.394607	-1225.260772	-1226.984224	-1226.589617
146-Int2	0.319217	-1032.355132	-1033.786678	-1033.467461
147-Int0	0.283826	-1373.974117	-1375.445725	-1375.161899
147-TS3	0.377647	-1568.047189	-1569.821968	-1569.444321
147-Int2	0.302783	-1375.137138	-1376.624038	-1376.321255
148-Int0	0.260728	-915.785138	-917.052653	-916.791925
148-TS3	0.355279	-1109.860434	-1111.427982	-1111.072703
148-Int2	0.280222	-916.951649	-918.231873	-917.951651
149-Int0	0.260841	-915.780788	-917.044903	-916.784062
149-TS3	0.356156	-1109.855609	-1111.420851	-1111.064695
149-Int2	0.279965	-916.946306	-918.225472	-917.945507
150-Int0	0.282071	-916.992494	-918.270715	-917.988644
150-TS3	0.378084	-1111.062928	-1112.648161	-1112.270077
150-Int2	0.301807	-918.152963	-919.448176	-919.146369
151-Int0	0.300860	-1031.221272	-1032.638755	-1032.337895
151-TS3	0.395391	-1225.293385	-1227.013717	-1226.618326
151-Int2	0.319646	-1032.381361	-1033.813439	-1033.493793
152-Int0	0.284091	-1373.980634	-1375.454553	-1375.170462
152-TS3	0.379166	-1568.055148	-1569.829959	-1569.450793
152-Int2	0.303450	-1375.144378	-1376.632659	-1376.329209
153-Int0	0.411246	-1446.600713	-1448.585833	-1448.174587
153-TS3	0.506056	-1640.669464	-1642.959947	-1642.453891
153-Int2	0.430548	-1447.755088	-1449.759677	-1449.329129
154-Int0	0.282209	-1117.109304	-1118.615226	-1118.333017
154-TS3	0.375278	-1311.181214	-1312.988296	-1312.613018
154-Int2	0.300667	-1118.262497	-1119.789125	-1119.488458
155-Int0	0.267966	-1210.063303	-1211.325604	-1211.057638
155-TS3	0.363046	-1404.132163	-1405.696923	-1405.333877
155-Int2	0.287457	-1211.218079	-1212.500203	-1212.212746
156-Int0	0.242811	-893.320205	-894.538148	-894.295337

156-TS3	0.338754	-1087.390485	-1088.913844	-1088.575090
156-Int2	0.262260	-894.478746	-895.714635	-895.452375
157-Int0	0.255051	-873.503395	-874.709198	-874.454147
157-TS3	0.351912	-1067.570638	-1069.081006	-1068.729094
157-Int2	0.275217	-874.664823	-875.887158	-875.611941
158-Int0	0.239373	-1216.283790	-1217.545666	-1217.306293
158-TS3	0.335913	-1410.352920	-1411.920127	-1411.584214
158-Int2	0.258681	-1217.442582	-1218.721771	-1218.463090
159-Int0	0.256595	-873.532614	-874.735917	-874.479322
159-TS3	0.351160	-1067.601364	-1069.106998	-1068.755838
159-Int2	0.274735	-874.690108	-875.910889	-875.636154
160-Int0	0.243461	-893.356315	-894.575636	-894.332175
160-TS3	0.338754	-1087.428020	-1088.951243	-1088.612489
160-Int2	0.262114	-894.515755	-895.751707	-895.489593
161-Int0	0.238752	-1216.290244	-1217.550144	-1217.311392
161-TS3	0.334561	-1410.360730	-1411.925411	-1411.590850
161-Int2	0.258237	-1217.448962	-1218.726690	-1218.468453
162-Int0	0.272599	-895.556388	-896.795090	-896.522491
162-TS3	0.368226	-1089.625672	-1091.167945	-1090.799719
162-Int2	0.291786	-896.715150	-897.971107	-897.679321
163-Int0	0.320507	-1124.181492	-1125.715175	-1125.394668
163-TS3	0.417097	-1318.255791	-1320.090057	-1319.672960
163-Int2	0.340453	-1125.346947	-1126.896836	-1126.556383
164-Int0	0.286498	-1046.804367	-1048.220378	-1047.933880
164-TS3	0.382857	-1240.873532	-1242.597311	-1242.214454
164-Int2	0.306259	-1047.964213	-1049.400585	-1049.094326
165-Int0	0.299487	-1026.981315	-1028.385922	-1028.086435
165-TS3	0.395224	-1221.049542	-1222.759625	-1222.364401
165-Int2	0.318125	-1028.145426	-1029.566397	-1029.248272
166-Int0	0.283525	-1369.767337	-1371.226014	-1370.942489
166-TS3	0.379735	-1563.836102	-1565.601933	-1565.222198
166-Int2	0.302572	-1370.926364	-1372.403647	-1372.101075
167-Int0	0.260241	-911.577638	-912.832550	-912.572309
167-TS3	0.356618	-1105.648815	-1107.207712	-1106.851094
167-Int2	0.279860	-912.739841	-914.009916	-913.730056
168-Int0	0.260518	-911.573004	-912.824707	-912.564189
168-TS3	0.356902	-1105.645803	-1107.202695	-1106.845793
168-Int2	0.279547	-912.735139	-914.004110	-913.724563
169-Int0	0.282233	-912.785413	-914.051916	-913.769683
169-TS3	0.376324	-1106.854210	-1108.421824	-1108.045500
169-Int2	0.300526	-913.943200	-915.227618	-914.927092
170-Int0	0.300255	-1027.015865	-1028.420569	-1028.120314
170-TS3	0.394488	-1221.084385	-1222.789928	-1222.395440
170-Int2	0.319196	-1028.170541	-1029.592480	-1029.273284
171-Int0	0.283900	-1369.773625	-1371.234951	-1370.951051
171-TS3	0.379327	-1563.845356	-1565.611176	-1565.231849
171-Int2	0.303099	-1370.933182	-1372.411226	-1372.108127
172-Int0	0.436718	-2658.605725	-2660.808782	-2660.372064
172-TS3	0.536146	-2852.676407	-2855.189555	-2854.653409
172-Int2	0.458682	-2659.762545	-2661.986221	-2661.527539
173-Int0	0.311079	-2329.109679	-2330.834220	-2330.523141
173-TS3	0.406968	-2523.186095	-2525.218776	-2524.811808
173-Int2	0.329333	-2330.270208	-2332.015520	-2331.686187
174-Int0	0.294386	-2422.066316	-2423.544956	-2423.250570
174-TS3	0.395279	-2616.136239	-2617.928981	-2617.533702
174-Int2	0.316238	-2423.225061	-2424.726170	-2424.409932
175-Int0	0.268237	-2105.326696	-2106.759648	-2106.491411
175-TS3	0.367758	-2299.397498	-2301.143668	-2300.775910
175-Int2	0.290769	-2106.488126	-2107.942679	-2107.651910
176-Int0	0.282871	-2085.507259	-2086.930675	-2086.647804

176-TS3	0.381162	-2279.578417	-2281.315474	-2280.934312
176-Int2	0.304561	-2086.671761	-2088.114009	-2087.809448
177-Int0	0.265982	-2428.289491	-2429.767888	-2429.501906
177-TS3	0.362529	-2622.361347	-2624.149688	-2623.787159
177-Int2	0.287322	-2429.450957	-2430.949486	-2430.662164
178-Int0	0.283961	-2085.536592	-2086.956992	-2086.673031
178-TS3	0.382118	-2279.606908	-2281.340437	-2280.958319
178-Int2	0.304848	-2086.695689	-2088.137178	-2087.832330
179-Int0	0.270963	-2105.361799	-2106.798697	-2106.527734
179-TS3	0.368644	-2299.434049	-2301.181937	-2300.813293
179-Int2	0.291726	-2106.522870	-2107.979310	-2107.687584
180-Int0	0.266350	-2428.295408	-2429.772873	-2429.506523
180-TS3	0.364471	-2622.366971	-2624.156798	-2623.792327
180-Int2	0.287743	-2429.456621	-2430.954218	-2430.666475
181-Int0	0.300797	-2107.561577	-2109.018418	-2108.717621
181-TS3	0.398066	-2301.633296	-2303.401666	-2303.003600
181-Int2	0.321642	-2108.723942	-2110.199301	-2109.877659
182-Int0	0.348477	-2336.185368	-2337.934657	-2337.586180
182-TS3	0.446193	-2530.263983	-2532.322299	-2531.876106
182-Int2	0.370540	-2337.356255	-2339.122712	-2338.752172
183-Int0	0.315529	-2258.807070	-2260.441943	-2260.126414
183-TS3	0.411206	-2452.881653	-2454.826509	-2454.415303
183-Int2	0.334667	-2259.972275	-2261.626339	-2261.291672
184-Int0	0.326629	-2238.985416	-2240.608246	-2240.281617
184-TS3	0.424371	-2433.057400	-2434.993139	-2434.568768
184-Int2	0.348242	-2240.150916	-2241.792755	-2241.444513
185-Int0	0.310906	-2581.771997	-2583.448717	-2583.137811
185-TS3	0.406594	-2775.844500	-2777.831054	-2777.424460
185-Int2	0.330790	-2582.934784	-2584.631022	-2584.300232
186-Int0	0.288087	-2123.583204	-2125.056508	-2124.768421
186-TS3	0.385822	-2317.658215	-2319.440387	-2319.054565
186-Int2	0.310202	-2124.748713	-2126.238449	-2125.928247
187-Int0	0.287668	-2123.579326	-2125.047145	-2124.759477
187-TS3	0.384552	-2317.654014	-2319.432651	-2319.048099
187-Int2	0.309538	-2124.743715	-2126.232240	-2125.922702
188-Int0	0.309183	-2124.789985	-2126.273430	-2125.964247
188-TS3	0.407187	-2318.860465	-2320.656265	-2320.249078
188-Int2	0.330437	-2125.948738	-2127.453812	-2127.123375
189-Int0	0.327202	-2239.019080	-2240.640443	-2240.313241
189-TS3	0.425825	-2433.089187	-2435.022403	-2434.596578
189-Int2	0.348246	-2240.177605	-2241.818921	-2241.470675
190-Int0	0.310692	-2581.776980	-2583.455052	-2583.144360
190-TS3	0.408307	-2775.852117	-2777.840373	-2777.432066
190-Int2	0.332223	-2582.941451	-2584.638694	-2584.306471
191-Int0	0.437565	-1490.055536	-1492.120323	-1491.682758
191-TS3	0.533896	-1684.126969	-1686.498062	-1685.964166
191-Int2	0.456647	-1491.215218	-1493.296016	-1492.839369
192-Int0	0.309608	-1160.562544	-1162.148951	-1161.839343
192-TS3	0.404765	-1354.636841	-1356.527748	-1356.122983
192-Int2	0.327851	-1161.722373	-1163.326011	-1162.998160
193-Int0	0.292803	-1253.519928	-1254.859556	-1254.566753
193-TS3	0.390640	-1447.588496	-1449.236997	-1448.846357
193-Int2	0.314813	-1254.676552	-1256.035952	-1255.721139
194-Int0	0.268813	-936.776351	-938.072812	-937.803999
194-TS3	0.365235	-1130.846554	-1132.448487	-1132.083252
194-Int2	0.289791	-937.937339	-939.250614	-938.960823
195-Int0	0.281354	-916.959342	-918.243867	-917.962513
195-TS3	0.378899	-1111.027821	-1112.620922	-1112.242023
195-Int2	0.302921	-918.122712	-919.422880	-919.119959
196-Int0	0.264999	-1259.739947	-1261.080129	-1260.815130

196-TS3	0.360693	-1453.810811	-1455.456244	-1455.095551
196-Int2	0.284556	-1260.902809	-1262.258601	-1261.974045
197-Int0	0.282407	-916.988481	-918.270421	-917.988014
197-TS3	0.379502	-1111.056698	-1112.646131	-1112.266629
197-Int2	0.302750	-918.147628	-919.446536	-919.143786
198-Int0	0.269170	-936.813673	-938.112031	-937.842861
198-TS3	0.364367	-1130.885420	-1132.487055	-1132.122688
198-Int2	0.289099	-937.975223	-939.288524	-938.999425
199-Int0	0.264276	-1259.746562	-1261.084514	-1260.820238
199-TS3	0.360168	-1453.818181	-1455.462660	-1455.102492
199-Int2	0.285500	-1260.908008	-1262.263093	-1261.977593
200-Int0	0.298427	-939.012967	-940.330147	-940.031720
200-TS3	0.394895	-1133.082652	-1134.707642	-1134.312747
200-Int2	0.319183	-940.174414	-941.507630	-941.188447
201-Int0	0.348477	-2336.185368	-2337.934657	-2337.586180
201-TS3	0.446193	-2530.263983	-2532.322299	-2531.876106
201-Int2	0.370540	-2337.356255	-2339.122712	-2338.752172
202-Int0	0.312802	-1090.259720	-1091.755057	-1091.442255
202-TS3	0.409085	-1284.329942	-1286.131601	-1285.722516
202-Int2	0.333605	-1091.421113	-1092.933978	-1092.600373
203-Int0	0.324907	-1070.437254	-1071.920413	-1071.595506
203-TS3	0.422029	-1264.506683	-1266.298622	-1265.876593
203-Int2	0.346312	-1071.601762	-1073.101116	-1072.754804
204-Int0	0.308847	-1413.223176	-1414.760145	-1414.451298
204-TS3	0.404956	-1607.293431	-1609.137547	-1608.732591
204-Int2	0.328898	-1414.385317	-1415.939493	-1415.610595
205-Int0	0.286499	-955.035232	-956.369100	-956.082601
205-TS3	0.382873	-1149.107084	-1150.746337	-1150.363464
205-Int2	0.306682	-956.200351	-957.546981	-957.240299
206-Int0	0.286318	-955.031094	-956.361297	-956.074979
206-TS3	0.381983	-1149.103086	-1150.737916	-1150.355933
206-Int2	0.306930	-956.194384	-957.540555	-957.233626
207-Int0	0.307804	-956.241412	-957.586491	-957.278687
207-TS3	0.404526	-1150.309910	-1151.962983	-1151.558457
207-Int2	0.328275	-957.400466	-958.762858	-958.434583
208-Int0	0.326190	-1070.471313	-1071.954526	-1071.628336
208-TS3	0.423061	-1264.539511	-1266.329187	-1265.906126
208-Int2	0.346150	-1071.629406	-1073.128212	-1072.782062
209-Int0	0.308670	-1413.230929	-1414.770088	-1414.461418
209-TS3	0.404828	-1607.303067	-1609.146778	-1608.741950
209-Int2	0.330476	-1414.392179	-1415.947773	-1415.617297
210-Int0	0.437899	-1485.847311	-1487.900326	-1487.462427
210-TS3	0.530952	-1679.917431	-1682.271154	-1681.740202
210-Int2	0.456668	-1487.003202	-1489.074006	-1488.617338
211-Int0	0.307703	-1156.357170	-1157.928370	-1157.620667
211-TS3	0.403174	-1350.426250	-1352.301617	-1351.898443
211-Int2	0.327578	-1157.509451	-1159.102605	-1158.775027
212-Int0	0.292429	-1249.312880	-1250.639731	-1250.347302
212-TS3	0.389690	-1443.377545	-1445.010860	-1444.621170
212-Int2	0.313769	-1250.465715	-1251.814227	-1251.500458
213-Int0	0.267833	-932.569222	-933.852938	-933.585105
213-TS3	0.364292	-1126.637086	-1128.227380	-1127.863088
213-Int2	0.289086	-933.725990	-935.028687	-934.739601
214-Int0	0.281276	-912.750851	-914.023350	-913.742074
214-TS3	0.378242	-1106.817006	-1108.395325	-1108.017083
214-Int2	0.302128	-913.911759	-915.201167	-914.899039
215-Int0	0.264600	-1255.532318	-1256.860264	-1256.595664
215-TS3	0.360182	-1449.600202	-1451.234992	-1450.874810
215-Int2	0.283706	-1256.691805	-1258.036464	-1257.752758

216-Int0	0.281545	-912.781798	-914.050900	-913.769355
216-TS3	0.378853	-1106.845941	-1108.420119	-1108.041266
216-Int2	0.302414	-913.936185	-915.224994	-914.922580
217-Int0	0.269236	-932.605031	-933.891431	-933.622195
217-TS3	0.364646	-1126.674613	-1128.264799	-1127.900153
217-Int2	0.288846	-933.763196	-935.066312	-934.777466
218-Int0	0.264049	-1255.538448	-1256.864127	-1256.600078
218-TS3	0.360641	-1449.607011	-1451.239329	-1450.878688
218-Int2	0.285158	-1256.696328	-1258.041298	-1257.756140
219-Int0	0.298531	-934.805138	-936.110620	-935.812089
219-TS3	0.393742	-1128.872793	-1130.481869	-1130.088127
219-Int2	0.319008	-935.962661	-937.286119	-936.967111
220-Int0	0.346291	-1163.430102	-1165.031406	-1164.685115
220-TS3	0.442130	-1357.503354	-1359.404099	-1358.961969
220-Int2	0.367290	-1164.594824	-1166.211589	-1165.844299
221-Int0	0.311831	-1086.053002	-1087.535022	-1087.223191
221-TS3	0.407520	-1280.121074	-1281.911020	-1281.503500
221-Int2	0.333055	-1087.210096	-1088.712540	-1088.379485
222-Int0	0.325749	-1066.229066	-1067.700517	-1067.374768
222-TS3	0.421114	-1260.296300	-1262.073702	-1261.652588
222-Int2	0.345405	-1067.391401	-1068.879908	-1068.534503
223-Int0	0.308992	-1409.015456	-1410.540415	-1410.231423
223-TS3	0.404055	-1603.084000	-1604.915179	-1604.511124
223-Int2	0.327818	-1410.174873	-1411.717746	-1411.389928
224-Int0	0.286173	-950.826165	-952.148425	-951.862252
224-TS3	0.381711	-1144.896590	-1146.521028	-1146.139317
224-Int2	0.306406	-951.988418	-953.325075	-953.018669
225-Int0	0.285817	-950.822123	-952.140555	-951.854738
225-TS3	0.383363	-1144.891808	-1146.516970	-1146.133607
225-Int2	0.306336	-951.983119	-953.319008	-953.012672
226-Int0	0.307221	-952.034059	-953.366077	-953.058856
226-TS3	0.403453	-1146.099429	-1147.736598	-1147.333145
226-Int2	0.327772	-953.189427	-954.541573	-954.213801
227-Int0	0.326213	-1066.264309	-1067.735710	-1067.409497
227-TS3	0.421595	-1260.329618	-1262.103326	-1261.681731
227-Int2	0.345873	-1067.418013	-1068.906601	-1068.560728
228-Int0	0.309169	-1409.022761	-1410.550470	-1410.241301
228-TS3	0.404027	-1603.093125	-1604.923410	-1604.519383
228-Int2	0.329183	-1410.181566	-1411.725906	-1411.396723

- The and $\mathbf{G_C}$ designate the Gibbs Free Energy at the M06-L/def2-SVP level.
- The and **G(gas)** designate Gibbs Free Energy in the gas phase at the M06-L/def2-SVP level.
- The $\mathbf{E_{SP} + G_{SOL}}$ designates the sum of single point energy at the M06-L/def2-TZVP level and the solvation free energy calculated by SMD continuum solvent mode.
- The **Final G** designates the sum of $\mathbf{E_{SP} + G_{SOL}}$ and $\mathbf{G_C}$.